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Title: Introduction to Interface Tracking in Multi-Material Flow Simulations

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Introduction to Interface Tracking in Multi-Material Flow Simulations

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Introduction

- Many real-world multi-physics applications also involve multiple materials
- Interesting physics occurs at material interfaces - surface tension, atomic mixing

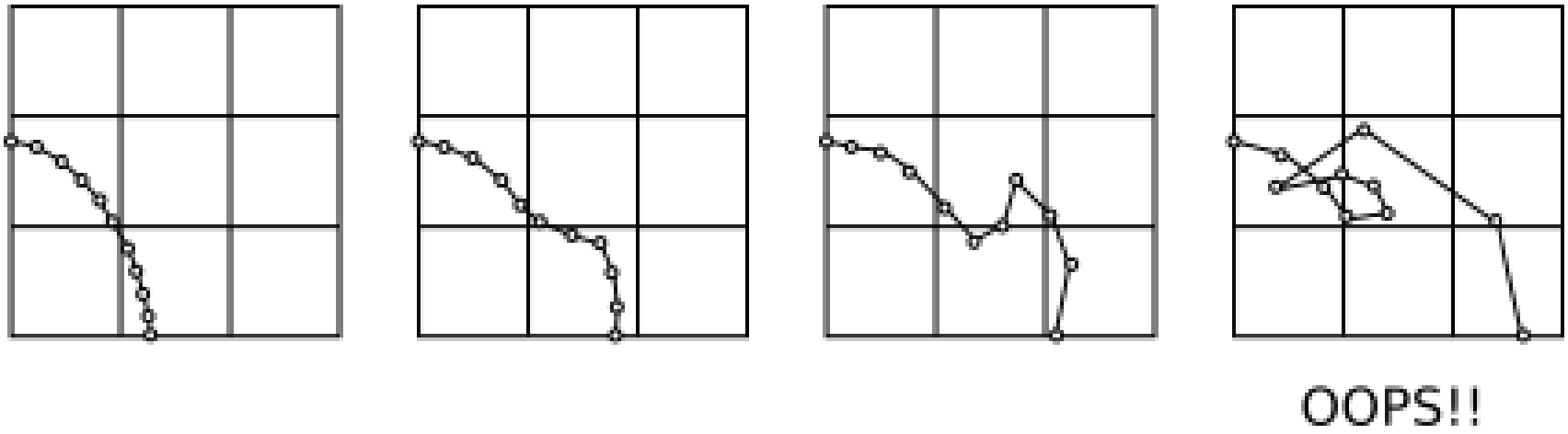
- Methods to track interfaces include:
  - *Front tracking methods* (Glimm, et.al.)
  - *Level set methods* (Osher and Sethian)
  - *Volume-of-fluid methods* (Hirt et. al.)
  - *Moment-of-fluid methods* (Dyadechko et. al.)

In this talk, I will predominantly discuss Volume-of-fluid and Moment-of-fluid methods.

Front tracking

- Interface is represented explicitly by a separate lower-dimensional mesh
- Velocities at interfacial points computed by interpolation from flow solution
- Points of interface moved at each time step using an accurate time-integration scheme
- Continuous interface makes calculation of interfacial area, curvature simple
- Captures subcell details better since the interfacial mesh can assume a complex shape within a cell

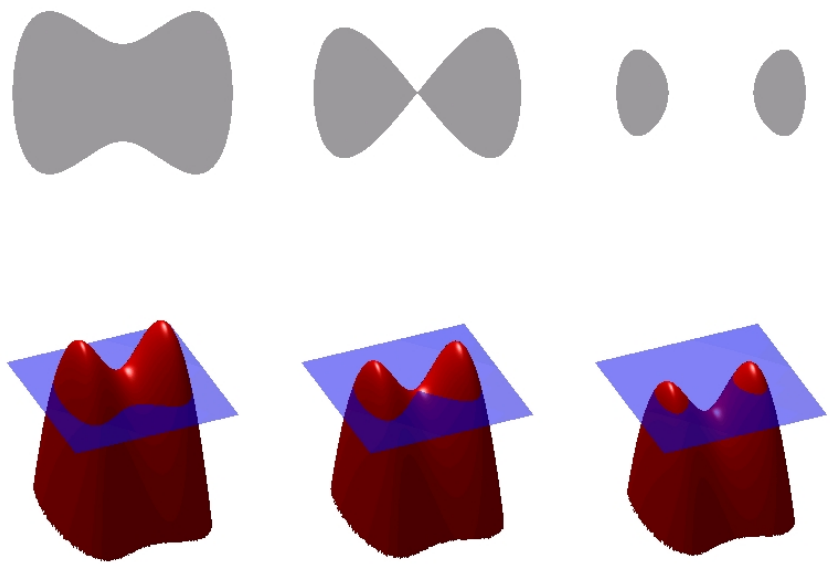
Front tracking (contd.)



- NO GUARANTEE of volume conservation
- Requires periodic "renormalization" - addition, deletion or redistribution of points from the interfacial mesh
- Topological changes in interface (break-up, merging) are non-trivial to implement particularly in 3D simulations

Level Set Methods

- Track the evolution of a closed, possibly multiply connected contour Γ
- Transform the problem to that of tracking evolution of a distance function ϕ whose zero level contour is Γ.
- ϕ is positive inside Γ, negative outside.



Source: Wikipedia

Level Set Method (contd.)

- Level Set Function is evolved using the Level Set Equation given by:

$$\frac{\partial \phi}{\partial t} = v|\nabla \phi|$$

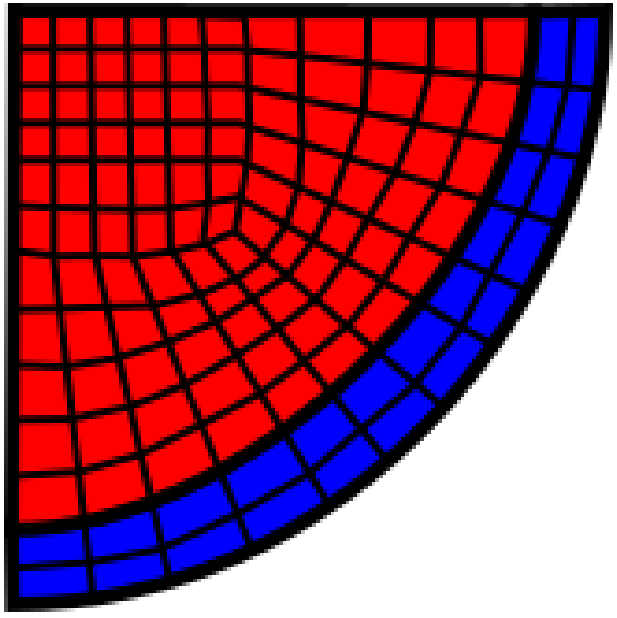
- v is normal velocity at any point on Γ
- Equation discretized and solved like any other partial differential euqaion in the system.
- Gives a smooth interface with no barriers to topology change (material break up, merging)
- Easy to compute curvature making it valuable for evolution of flame or shock fronts as well as computation of surface tension
- NO GUARANTEE of volume conservation
- Problems for N materials ($N > 2$) - Need $N - 1$ level set functions; Gaps at multi-material junctions

Volume-of-fluid Methods

Volume-of-Fluid or VOF Method

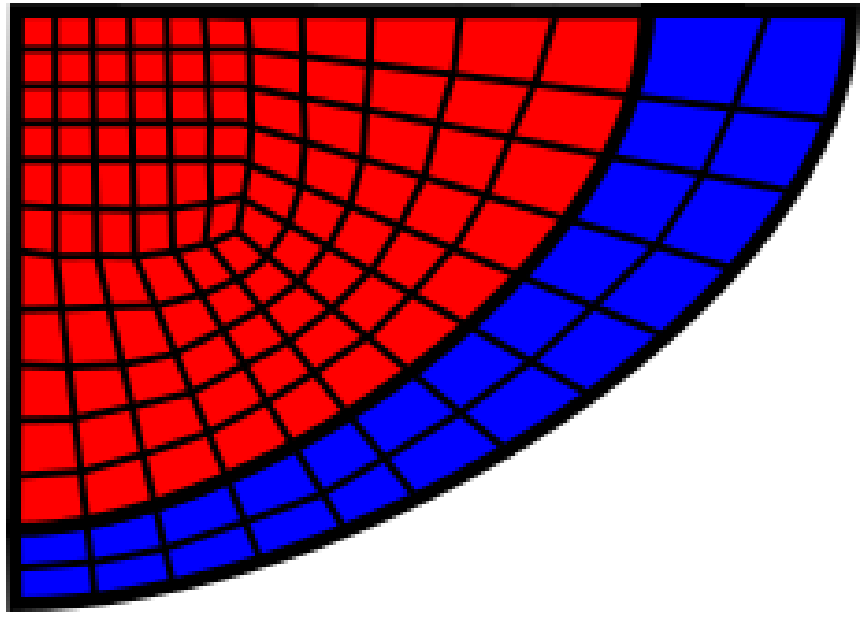
- Pioneered by Hirt and Nichols
- Tracks relative volumes or volume fractions of multiple materials in cells
- No explicit tracking of interfacial surfaces
- Cells with one material are called PURE, with multiple materials are called MIXED
- Interfacial curves/surfaces are reconstructed from volume fractions in MIXED cells only when necessary
- By definition, method strictly conserves mass of individual fluids

Mesh will have only PURE cells –IF–



Initial mesh aligned with material interfaces

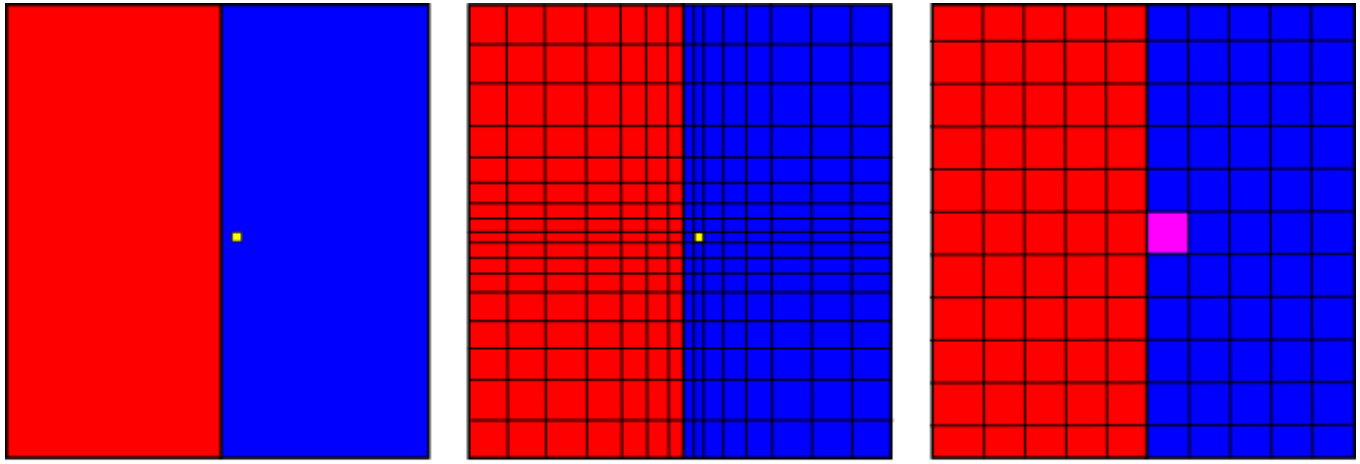
AND



Mesh moves with material

Mesh has Mixed Cells –IF–

- Problem has some relatively small but important material parts
- Explicitly meshing these small parts would need very small element sizes around features
  – increase in number of elements
  – dropping of time step due to CFL condition
- Instead we create larger cells that are mixed to account for the different materials



Domain with small feature in yellow

Small feature captured by refinement

Small feature absorbed into large mixed cell

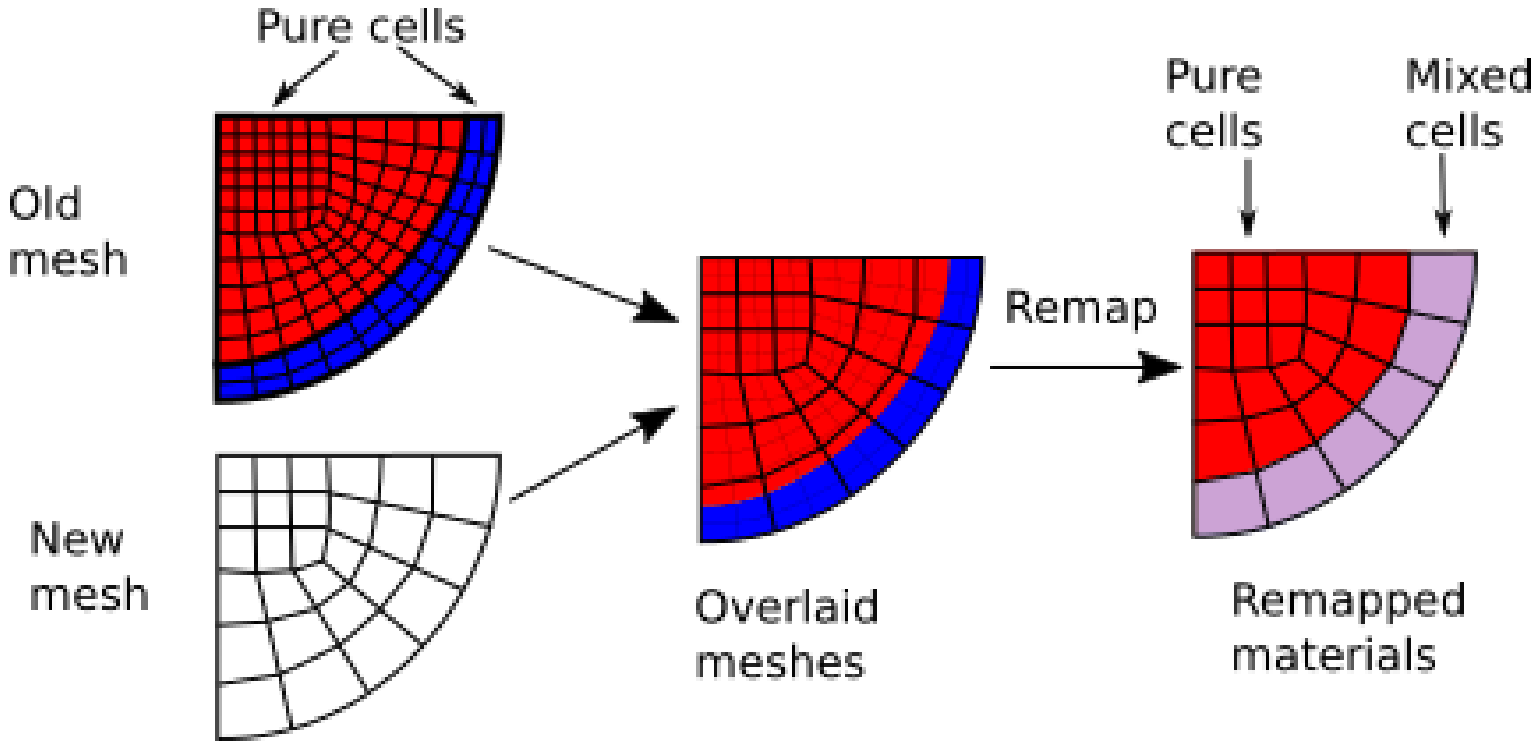
Mesh has Mixed Cells –IF–

- We REMAP simulation data to new mesh that is NOT ALIGNED with material interfaces
- Some new cells may overlap old mesh cells of different materials
- To be accurate, new cells must keep track of multiple materials making it mixed

- New mesh may be due to modification of current mesh ignoring material interfaces
- Done to prevent tangling due to Lagrangian motion (Arbitrary-Lagrangian-Eulerian methods)

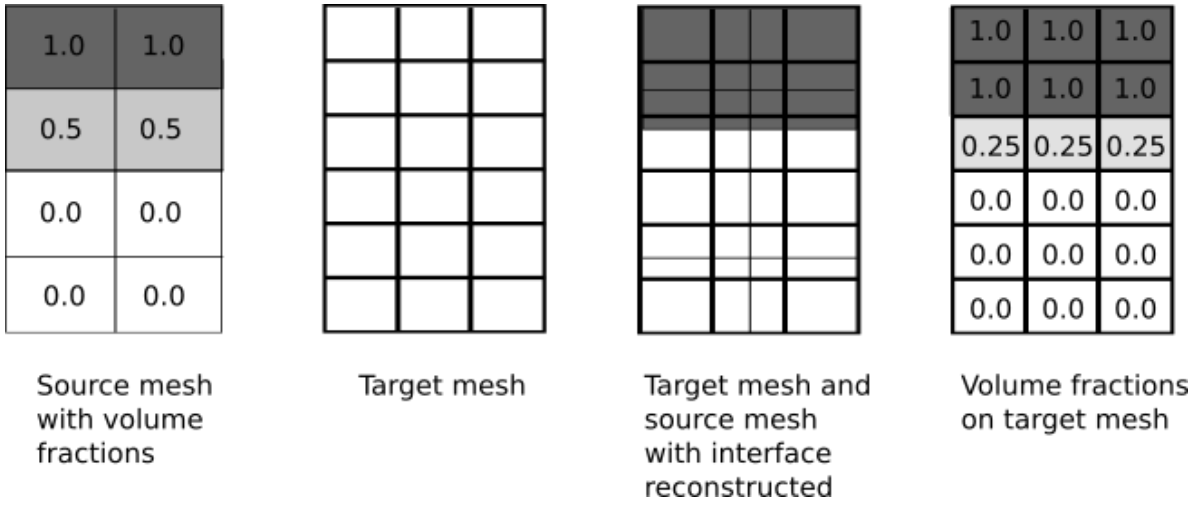
- New mesh may also be from a different physics module or even a different code

Mixed Cell Creation due to Remap

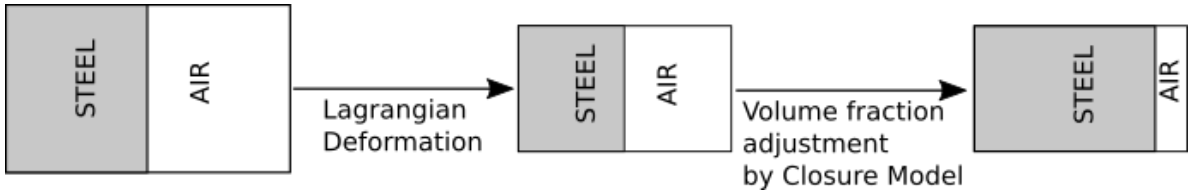


Why Reconstruct Interfaces from Volume Fractions?

- Remapping - accurate accounting of which pure material polygons intersect target mesh cells

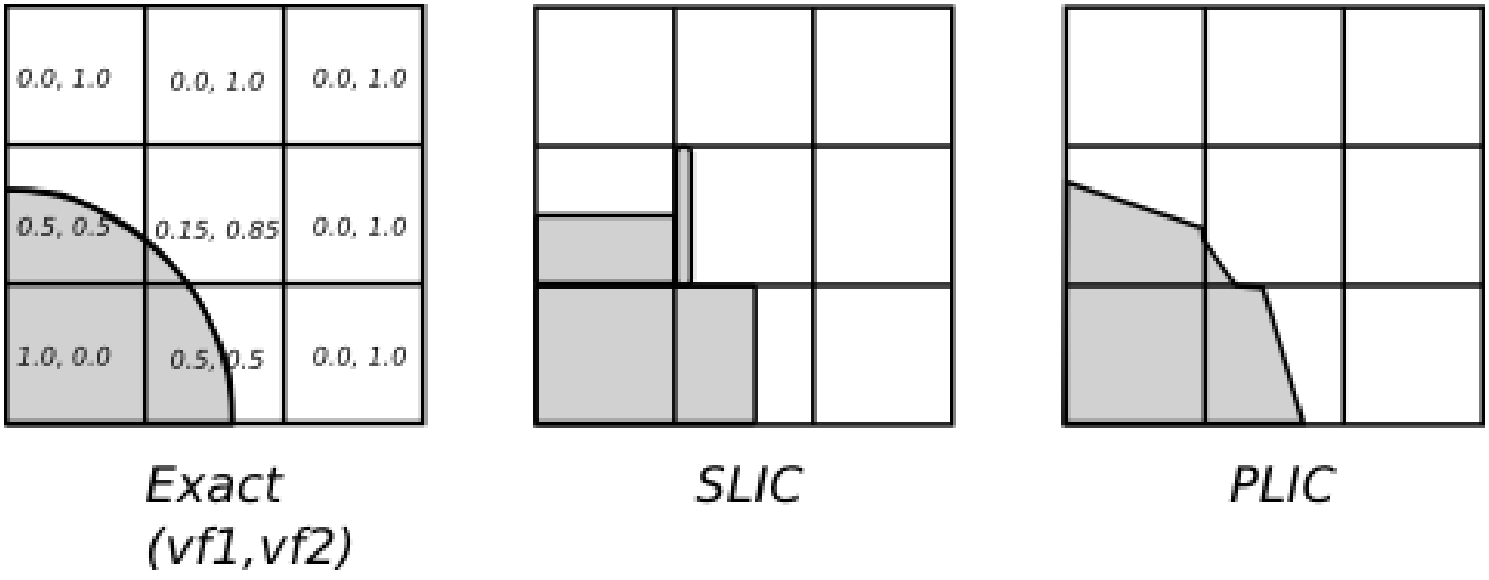


- Closure Models - accounting for difference material compressibility during Lagrangian deformation



- Multi-material Diffusion - More accurate solution of diffusion by avoiding homogenization of properties

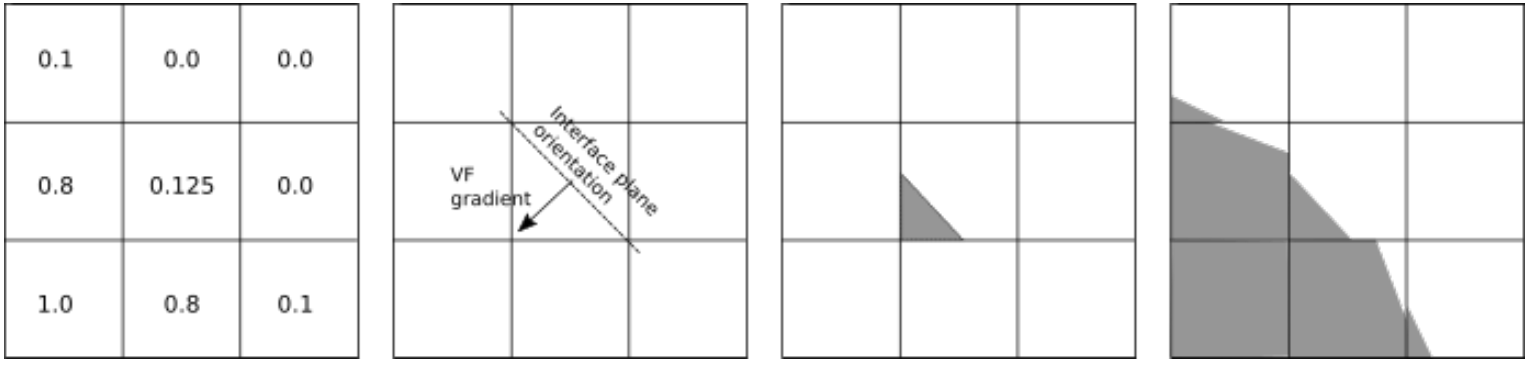
Reconstruction of Interfaces from Volume Fractions



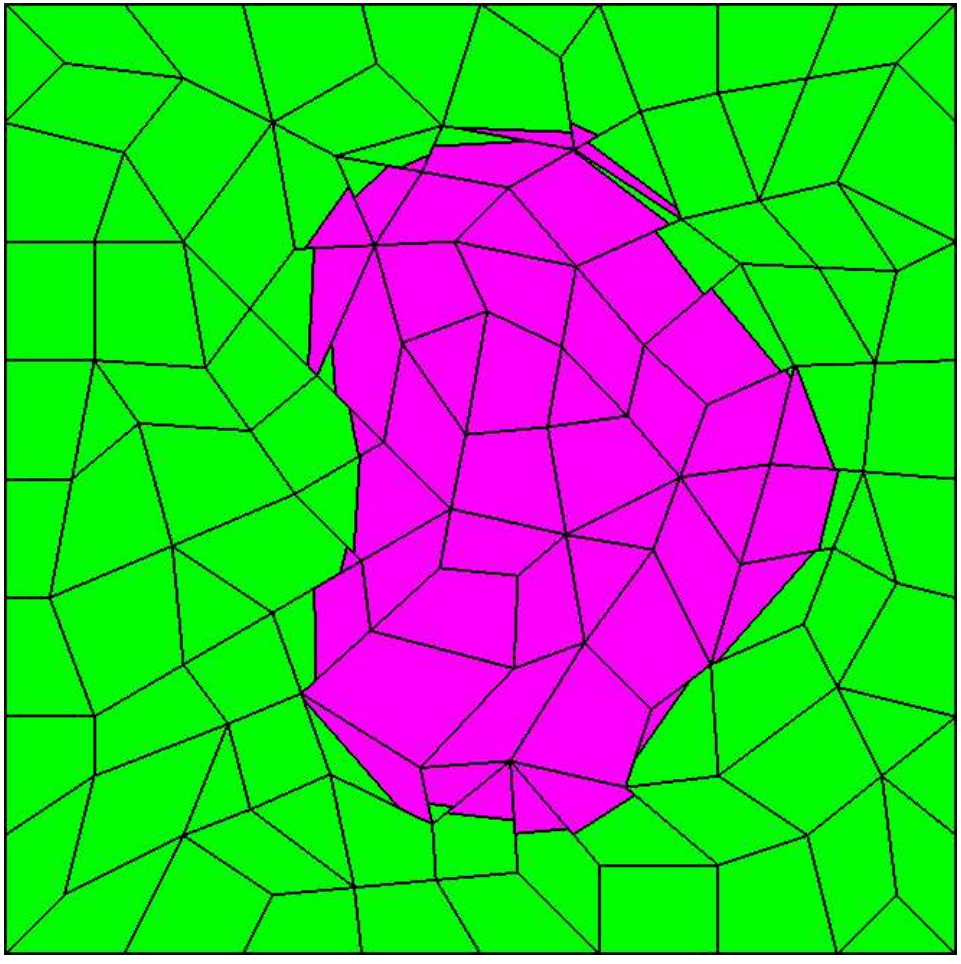
- Early codes reconstructed interface in each cell as a straight line parallel to a coordinate axis (SLIC)
- D.L. Youngs introduced the notion of arbitrarily oriented piecewise linear interface (named PLIC by Rider and Kothe)
- Reconstruction of curved interfaces? Not common/robust

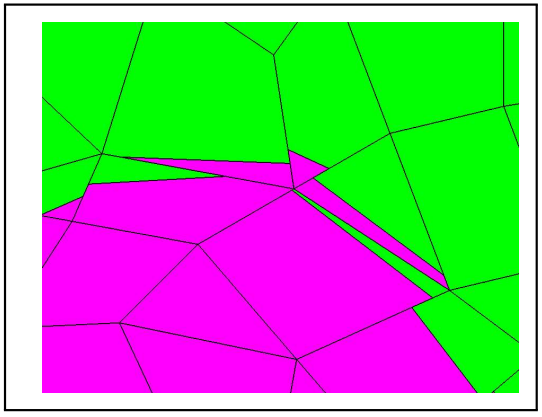
Gradient-Based Interface Reconstruction

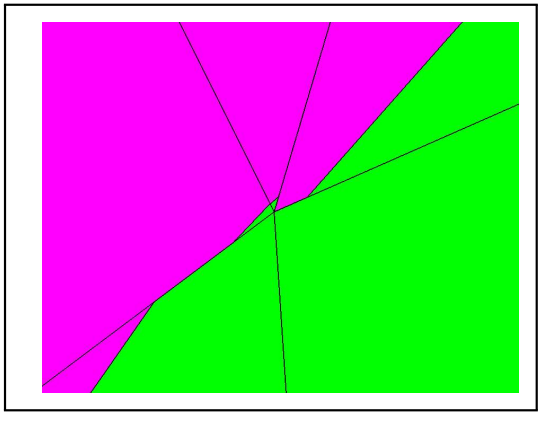
- View material volume fractions as values of a pseudo-density function specified at cell centers
- Compute gradient of the volume fraction function (typically by least squares fit of a linear function to the data)
- Interface normal — negative of volume fraction gradient
- Interface tangent line/plane segment is orthogonal to normal
- Move interface line along normal to get right volume fraction
- Gradient-based methods are generally first-order accurate



Interface Estimation



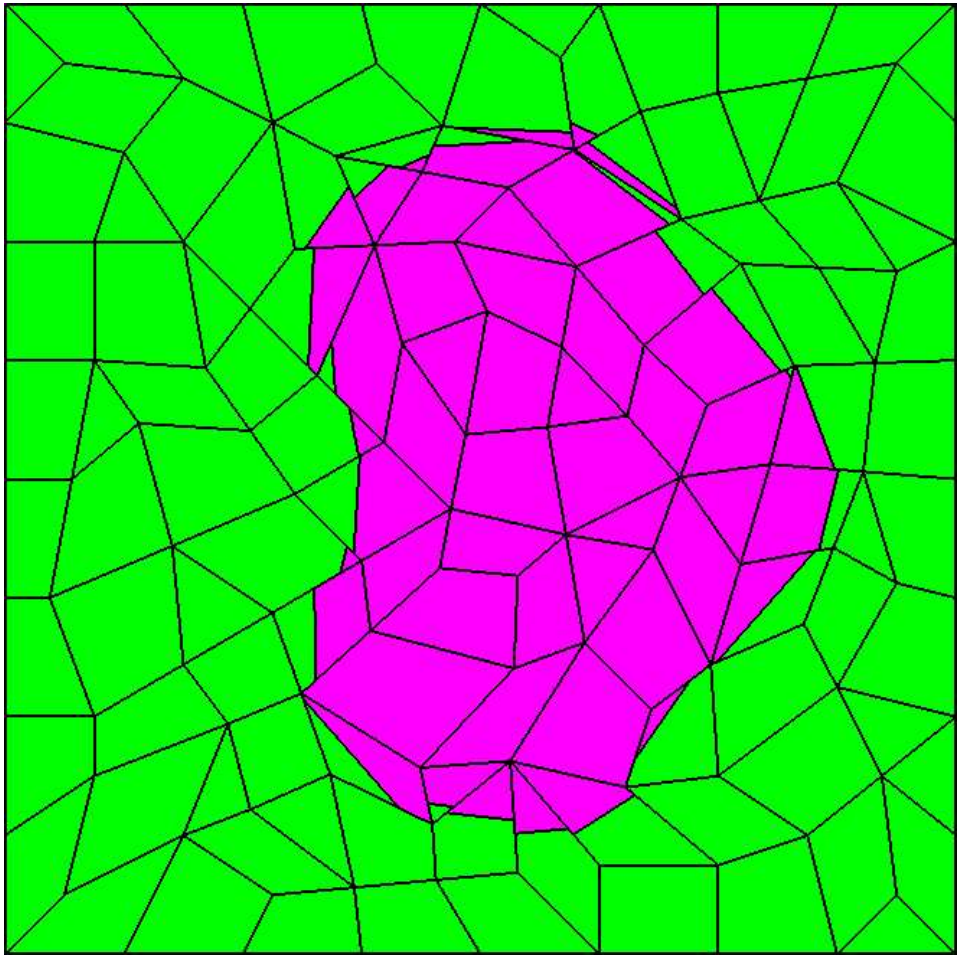


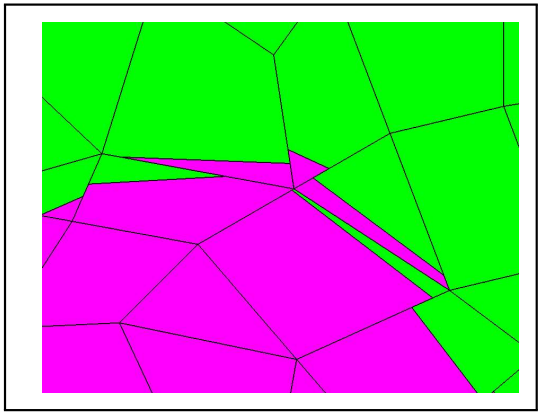


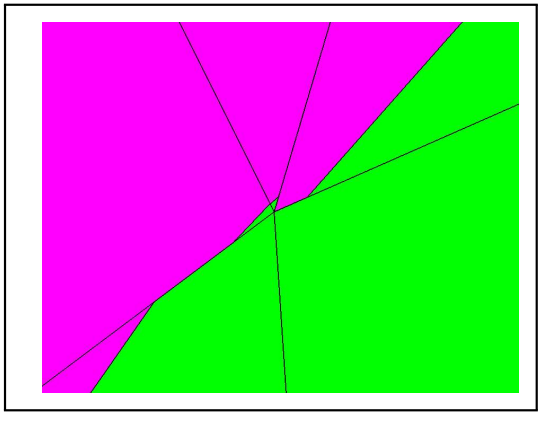
Second-Order Accurate Reconstruction or Interface Smoothing

- Swartz's method:
  - Find common line (plane) that cuts off exact volume fraction in cell and each mixed cell neighbor (Steinhaus theorem on "Ham Sandwich Problem")
  - New normal – average of normals to all such lines
  - Reposition interface to cut off the right volume fraction
- LVIRA method:
  - Find interface normal that cuts off the exact volume fraction in cell while minimizing error in neighboring mixed cells
  - More easily generalizable than Swartz's method to 3D
- Needs reasonable initial guess (from interface estimation)
- Second order convergence

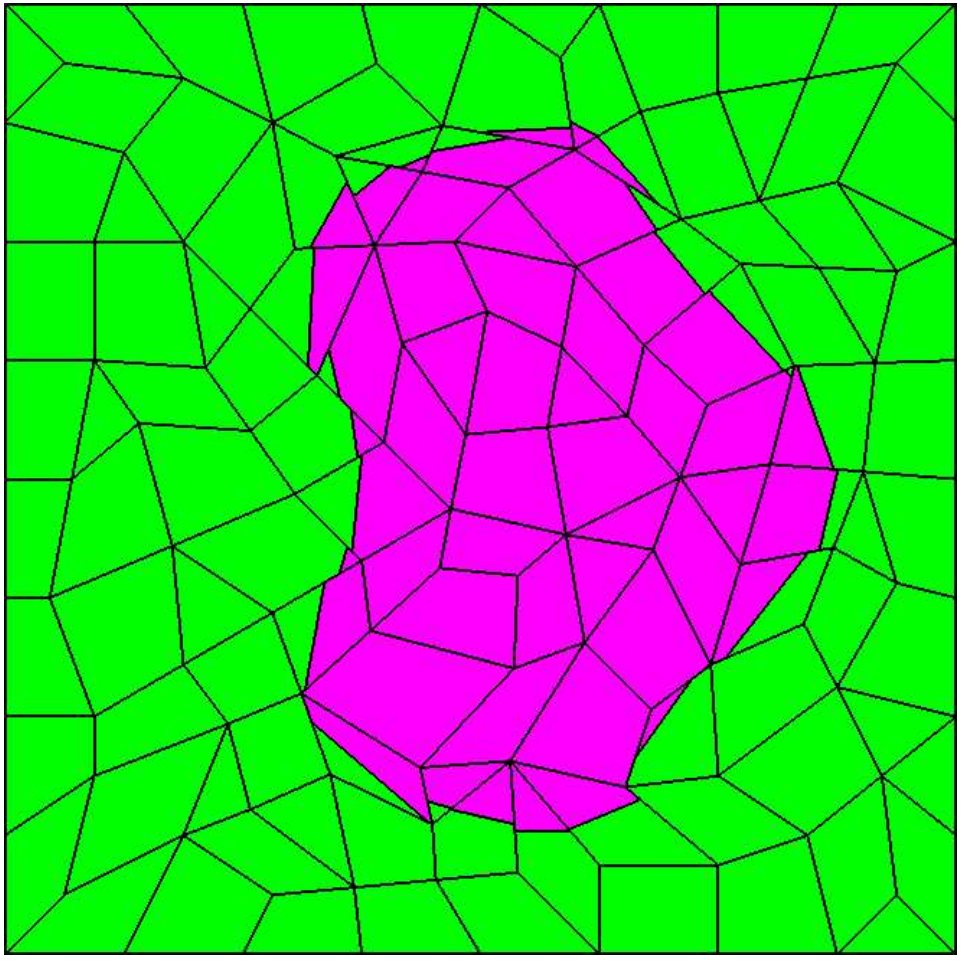
Interface Estimation

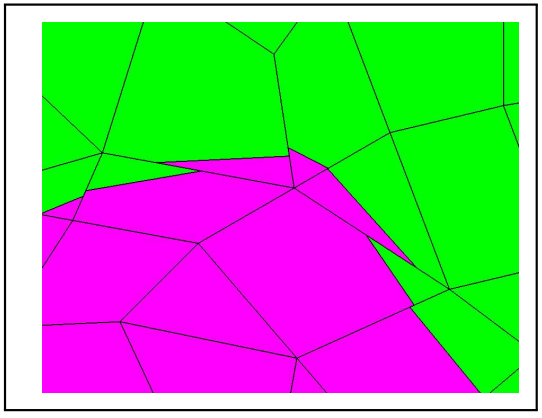


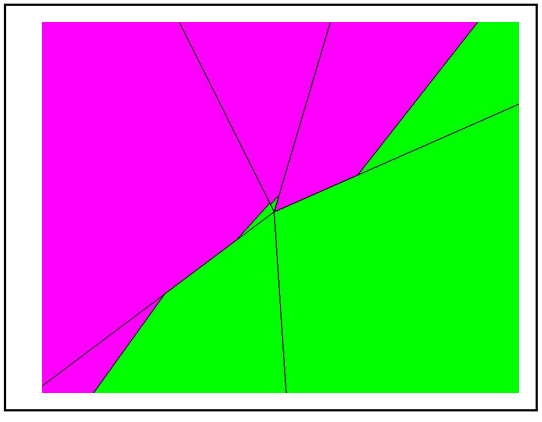




Interface Smoothing





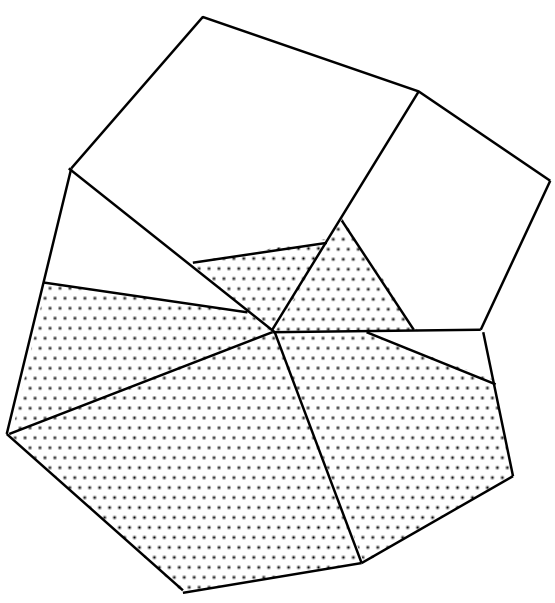


Topological Consistency and Repair of Interfaces

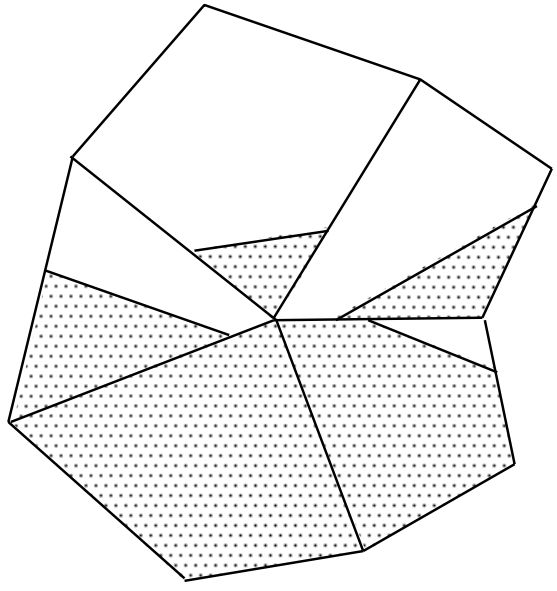
If we superimpose a closed shape on a mesh, every vertex must be inside, outside or on the boundary of the shape

Impose same criterion on interface reconstruction (as far as possible)

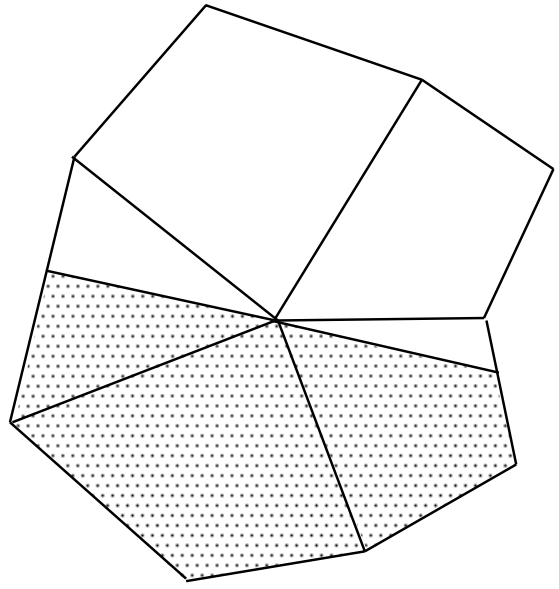
Tweak interfaces such that every vertex is inside the same material in all surrounding cells



Consistent

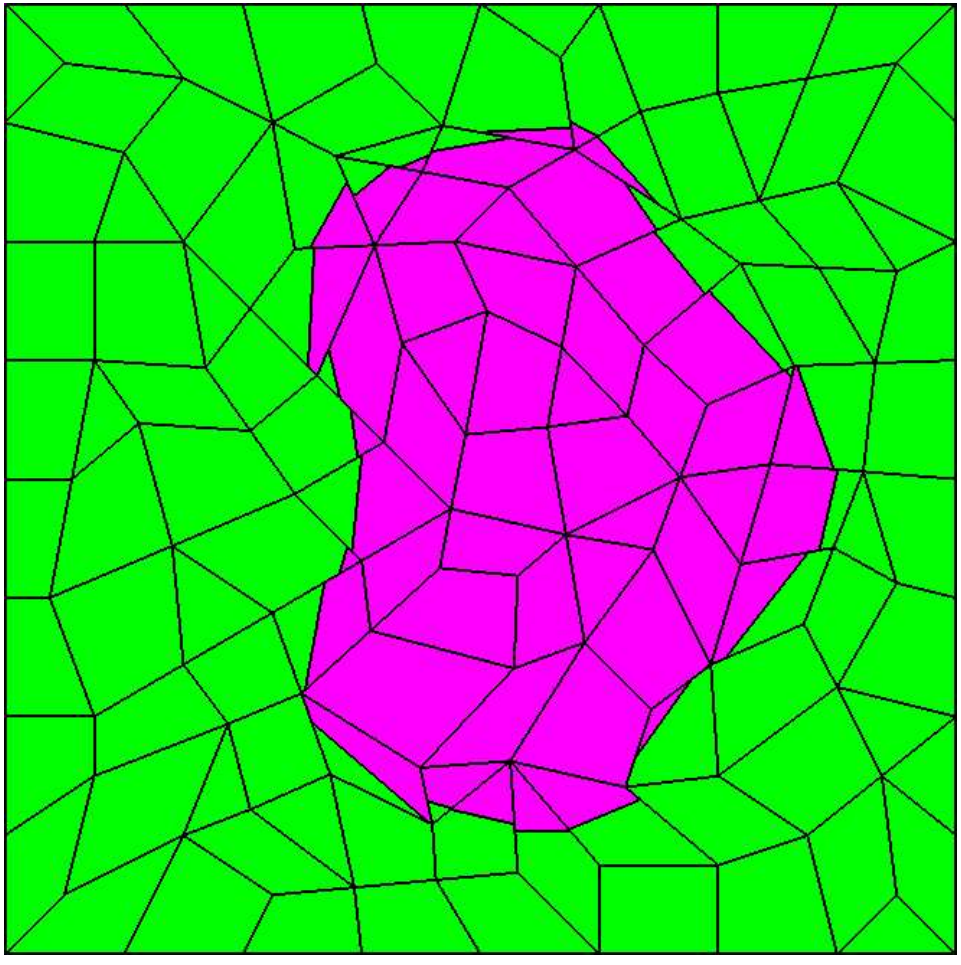


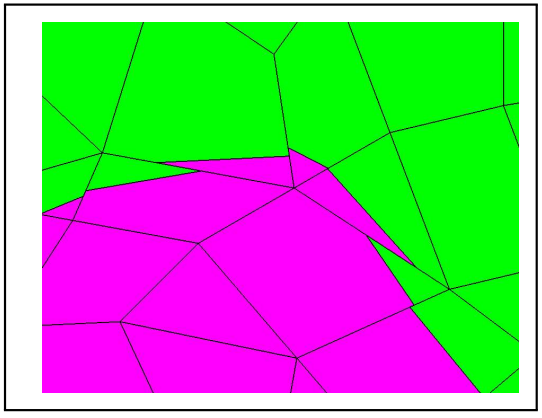
Inconsistent

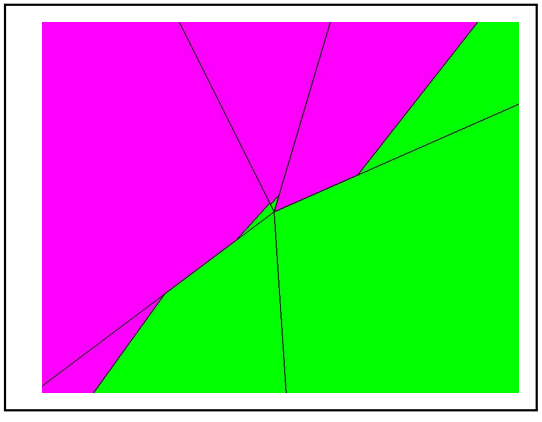


Ambiguous

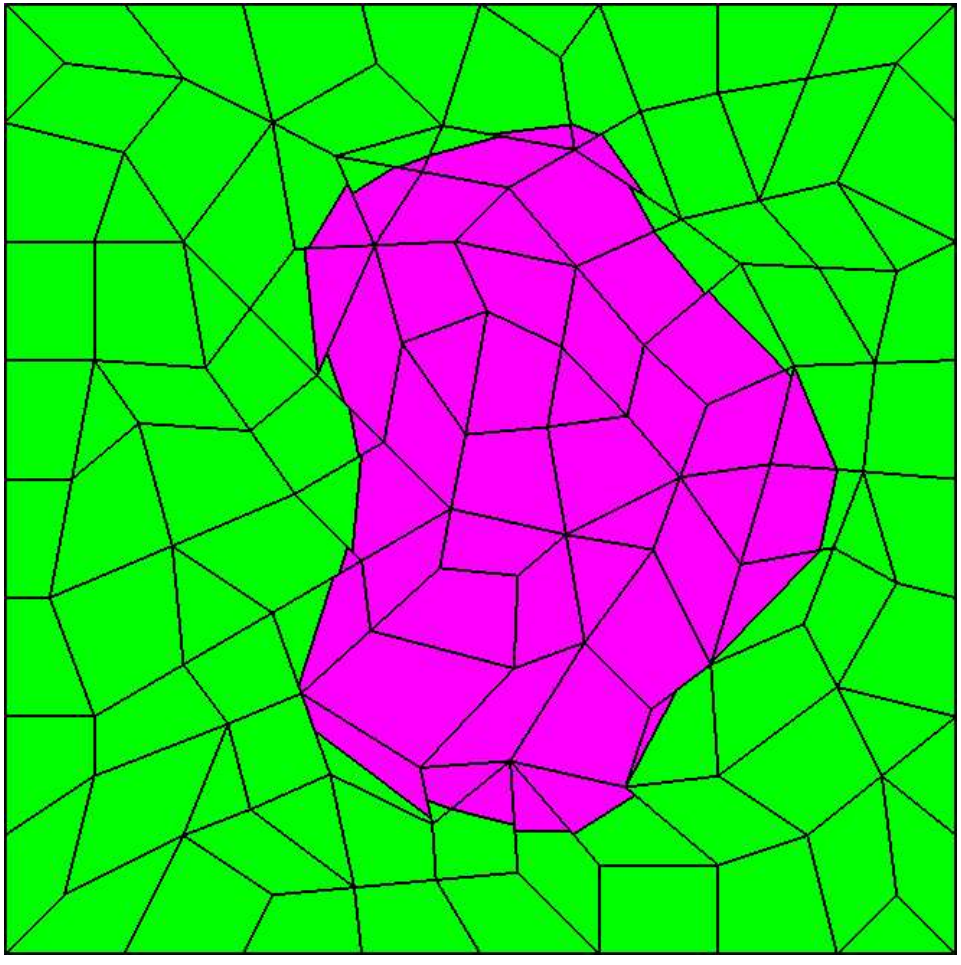
Interface Smoothing

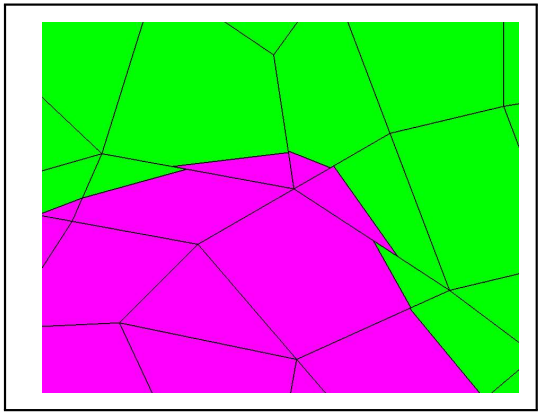


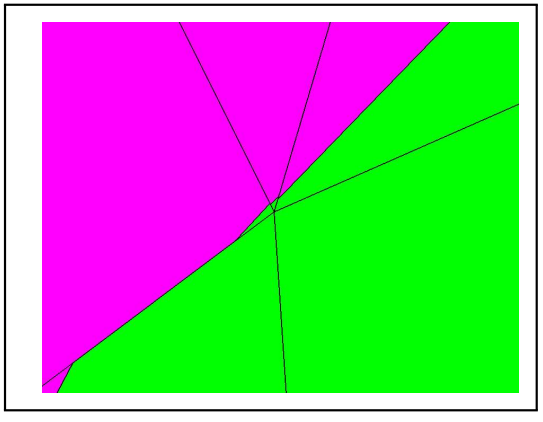




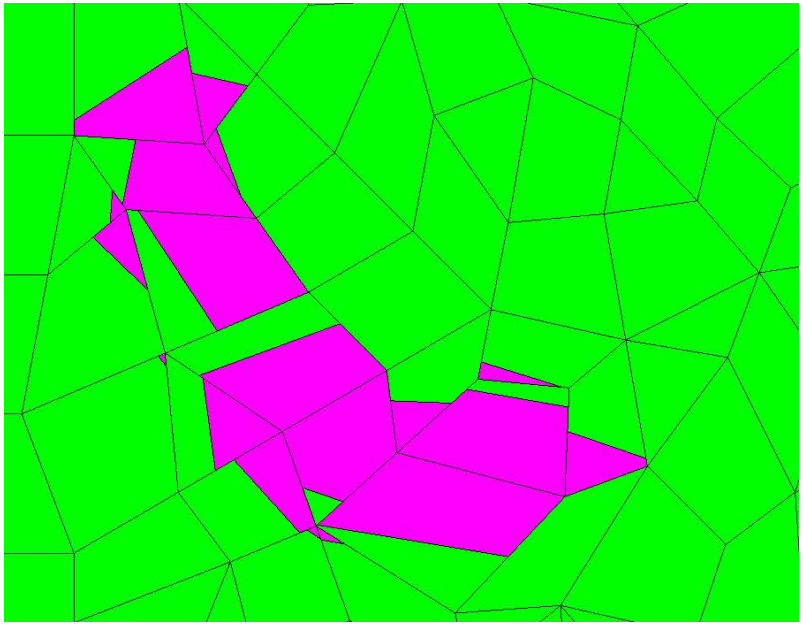
Topological Repair of Interface



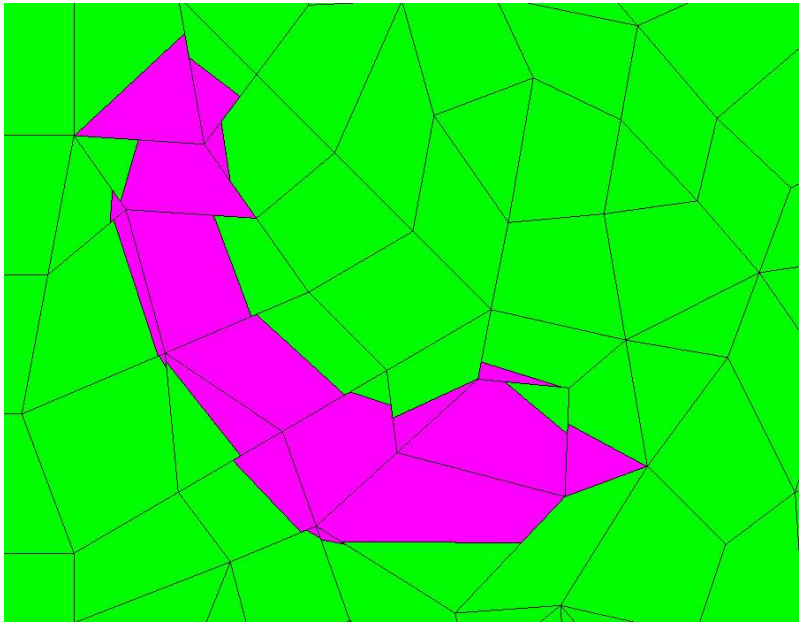




Topological Repair - Example 2



Before

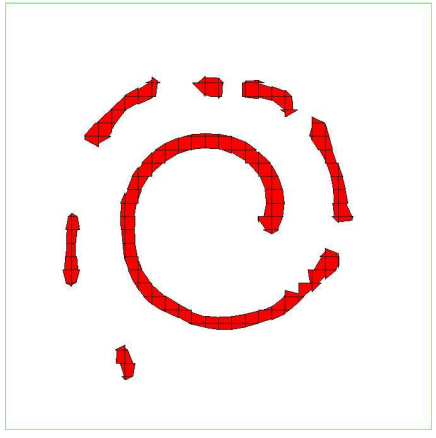


After

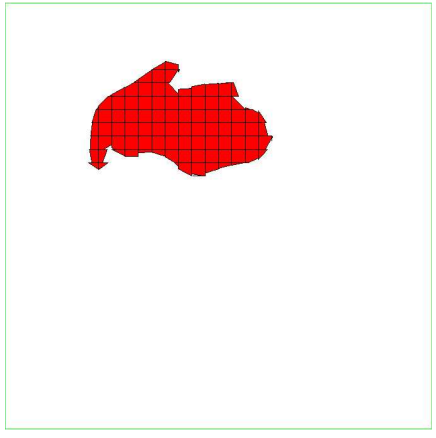
Example - Vortex-in-a-box (Rider and Kothe)

Analytical velocity profile given by the stream function with time reversal $\Psi = \frac{1}{\pi}\sin^2(\pi x)\sin^2(\pi y)cos(\pi t/T)$

32x32 grid

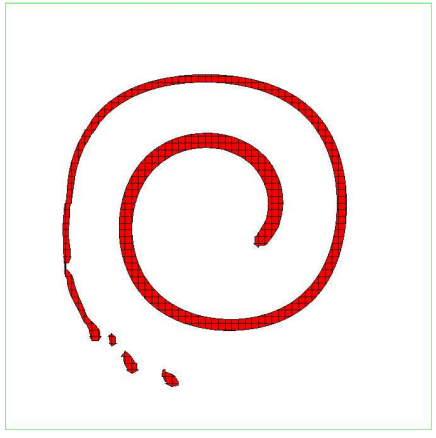


Maximal Stretch

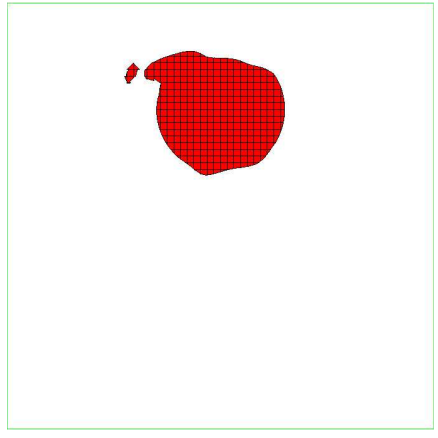


Fully Reversed

64x64 Grid

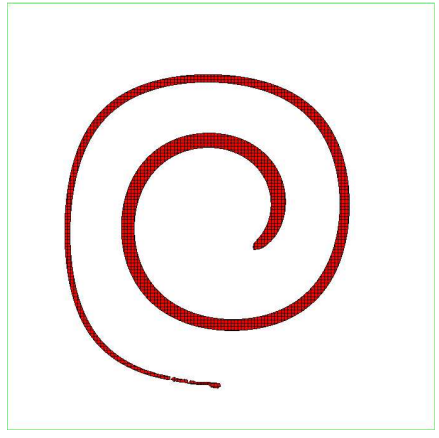


Maximal Stretch

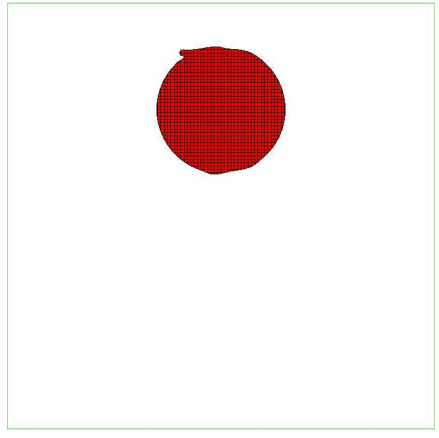


Fully Reversed

128x128 Grid

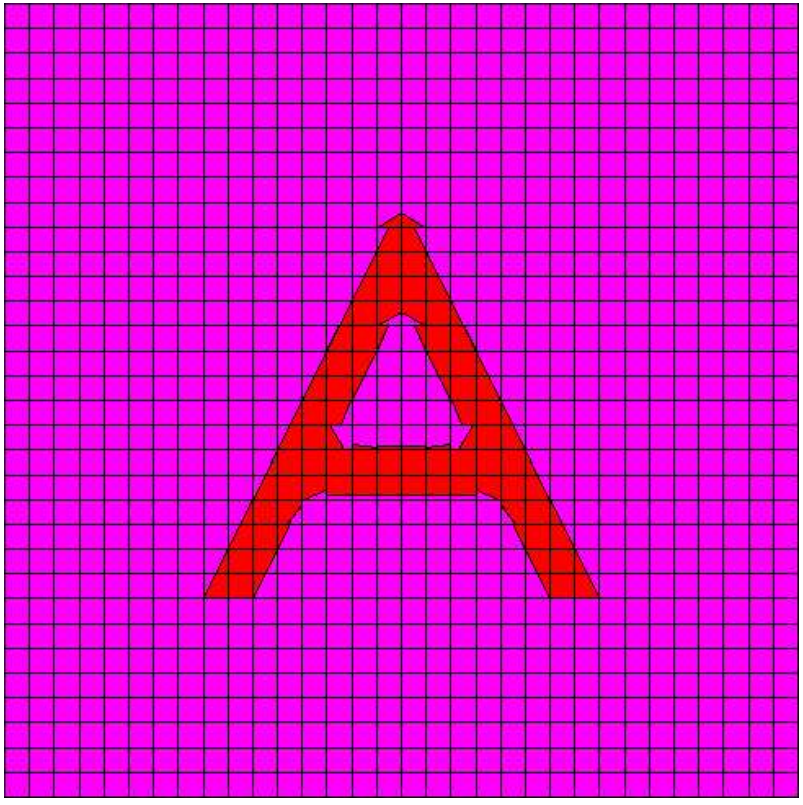


Maximal Stretch

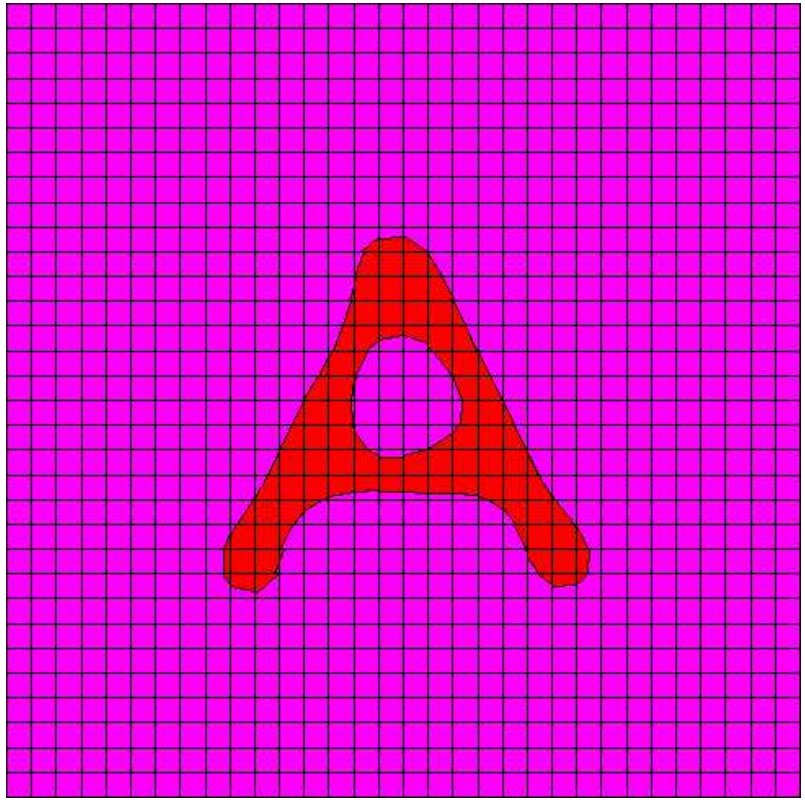


Fully Reversed

Letter “A” Rotation



Initial



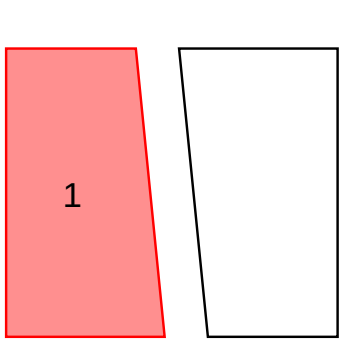
Final

Material-order-independent Reconstruction

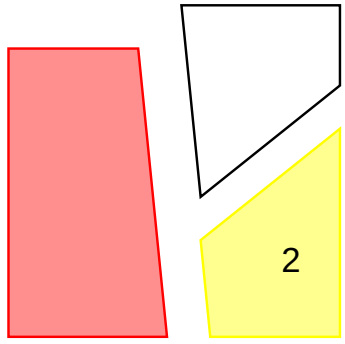
Material-Order-Dependence in VOF

- Multi-material (> 2) interface reconstruction presents challenges
- At best, VOF methods perform a nested dissection of cells
- In this method, the interface between the first material and the rest of the materials is found as usual
- This material is then carved off from the cell
- Then the next material is carved off from the remaining part of the cell
- The process continues until all materials have been carved off
- Clearly, the end result is highly dependent on the order in which materials are processed

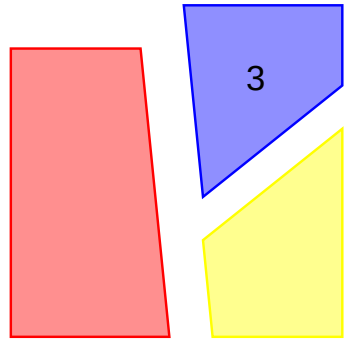
Nested dissection



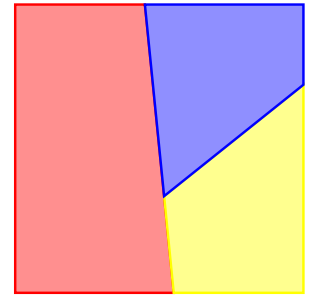
(a)



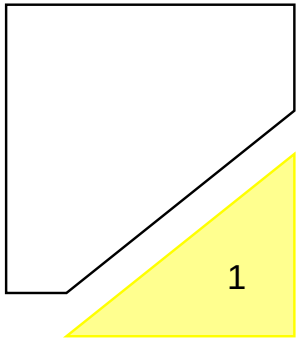
(b)



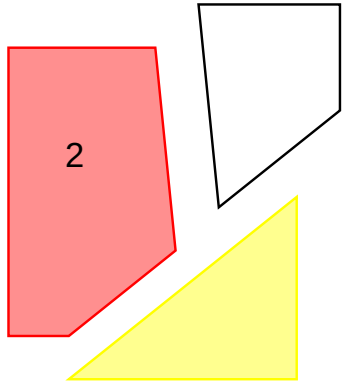
(c)



(d)



(e)



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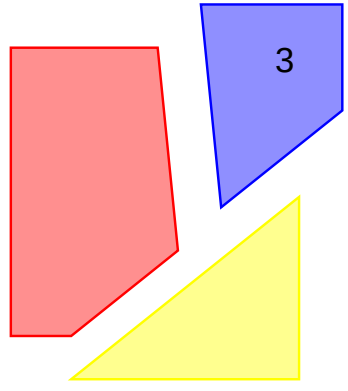
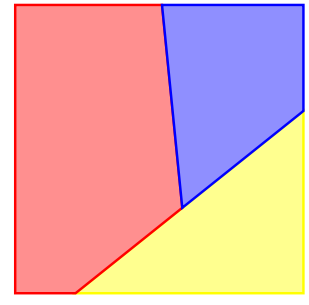
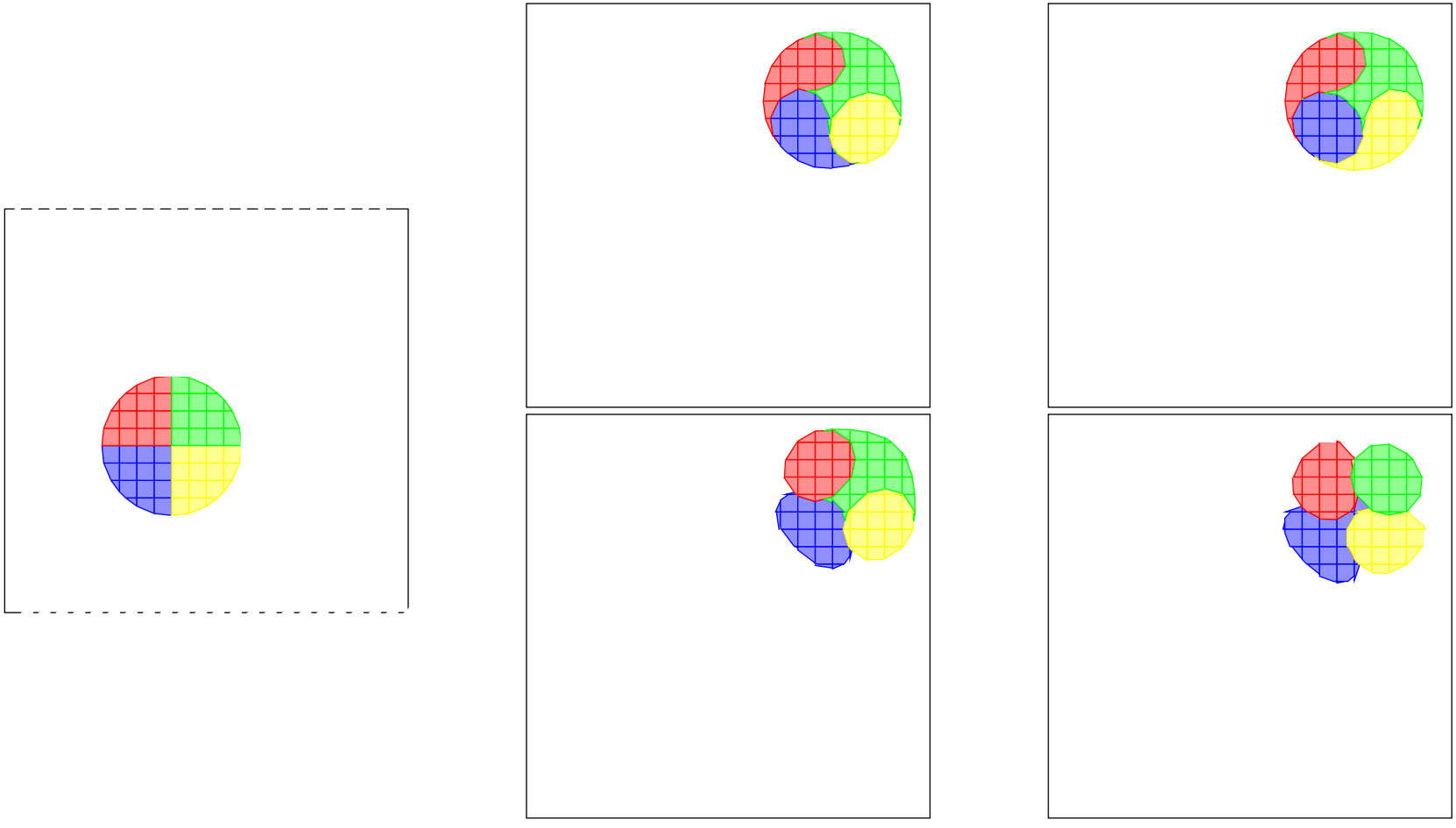


(g)



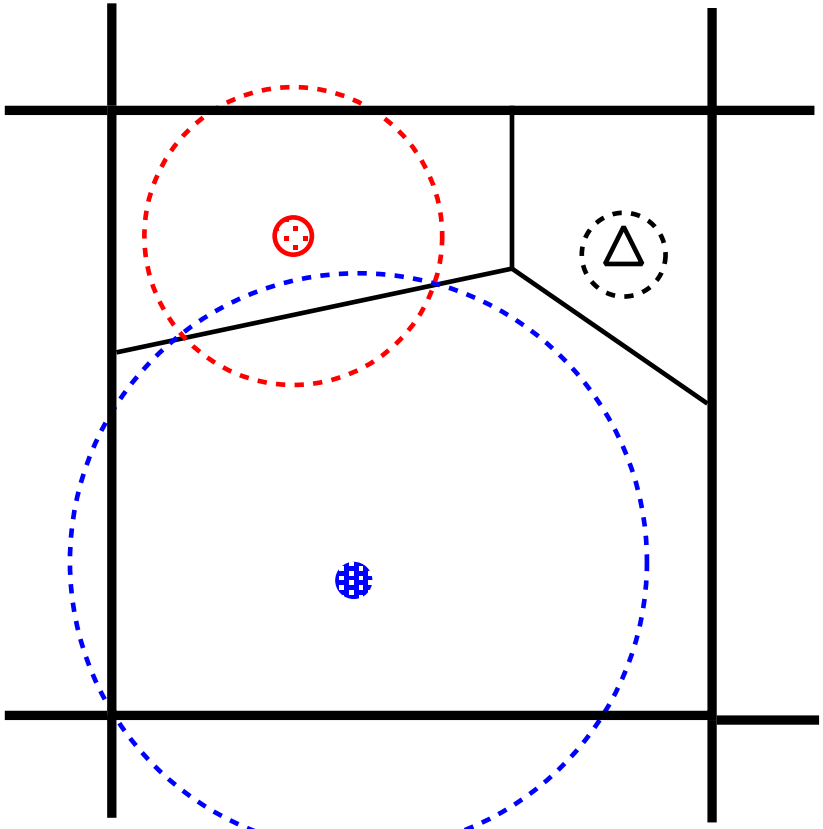
(h)

Consequences of Material-Order-Dependent Reconstruction

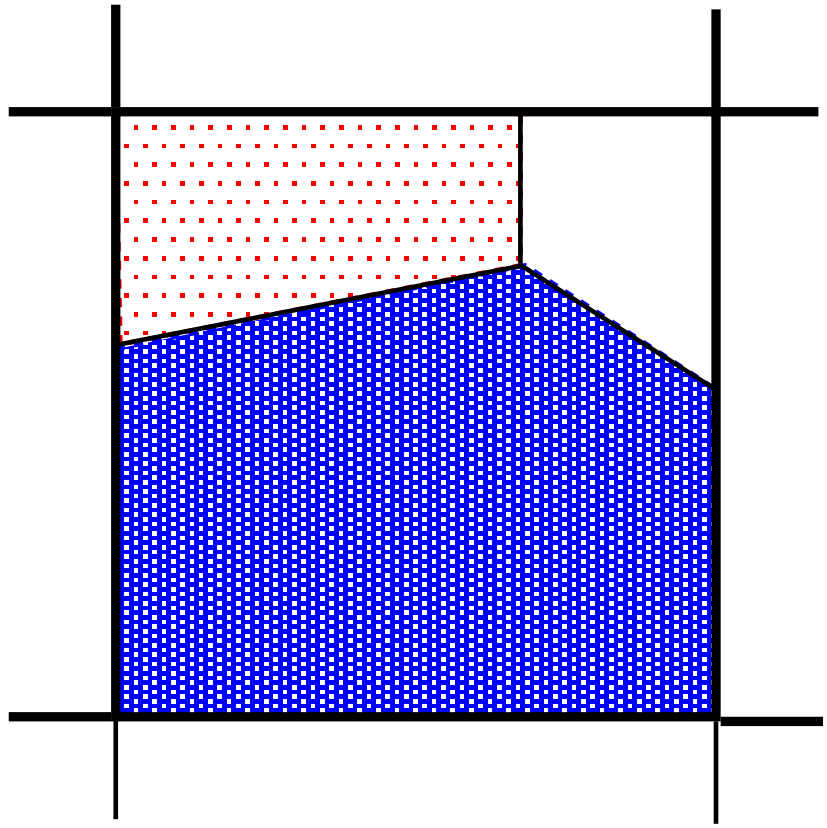


VOF-PD - Materia-Order-Independent Interface Reconstruction

Determine approximate material centroids in the cell by linear reconstruction of volume fraction functions



Subdivide cell using a weighted Voronoi (power) diagram



(d)

Material Location by Linear Reconstruction

- View volume fraction of material f_i^m as cell-centered value of pseudo-density function $\xi^m(\mathbf{x})$
- Compute linear reconstruction of pseudo-density function in cell

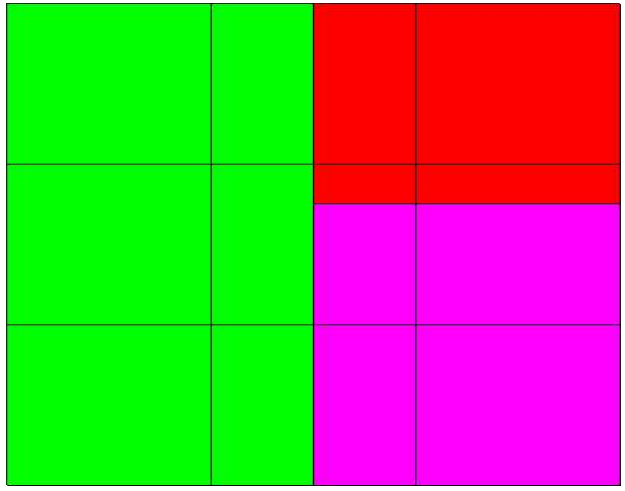
$$\xi^m(\mathbf{x}) = f_i^m + \boldsymbol{\delta}(\mathbf{x} - \bar{\mathbf{x}}_i)$$

- $\boldsymbol{\delta}$ is either Green-Gauss or Least Squares Gradient of ξ^m
- Gradient is limited so that no new extrema are created (Barth-Jesperson type limiter, limits [0.0,1.0])
- Approximate material centroid in the cell is computed by

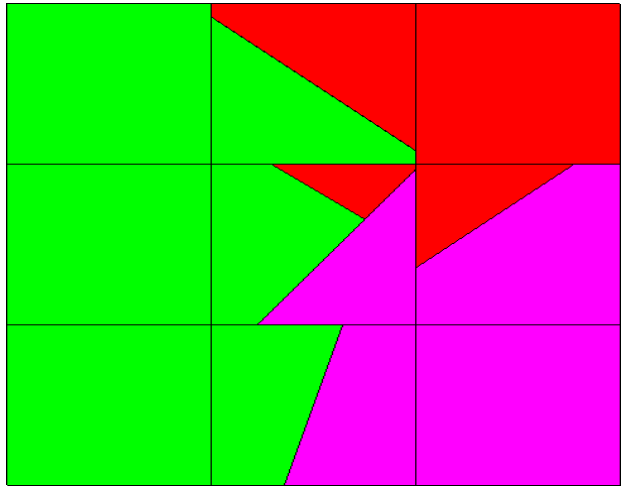
$$\bar{\mathbf{x}}_i^m = \frac{\int_\Omega \xi^m(\mathbf{x})\mathbf{x}d\mathbf{x}}{\int_\Omega \xi^m(\mathbf{x})d\mathbf{x}} = \frac{\int_\Omega \xi^m(\mathbf{x})\mathbf{x}d\mathbf{x}}{\|\Omega\| f_i^m}$$

Simple Example - Three Materials, Structured Grid

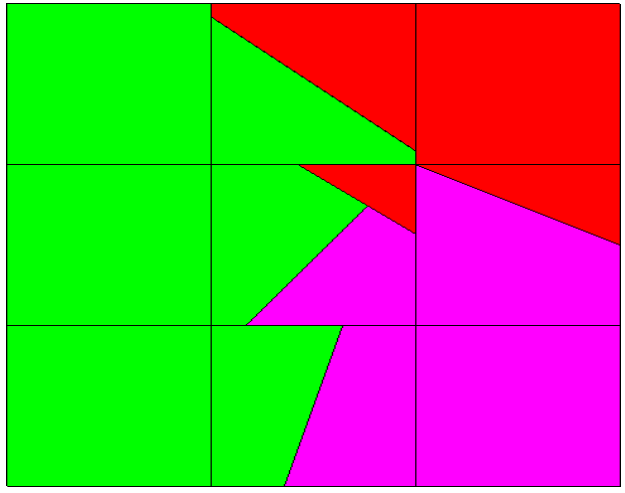
Gradient method
Ordering 0



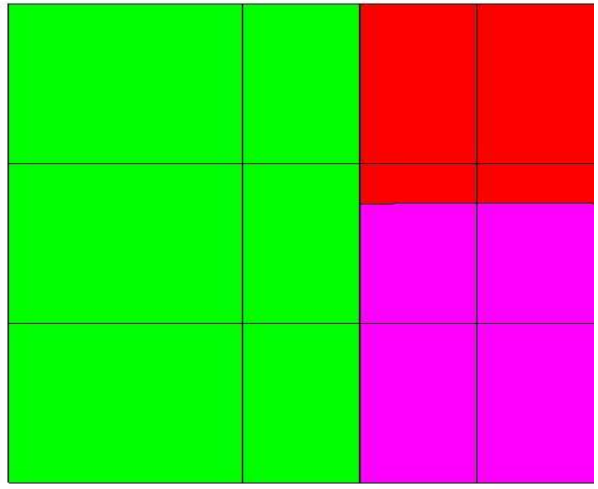
Gradient method
Ordering 1



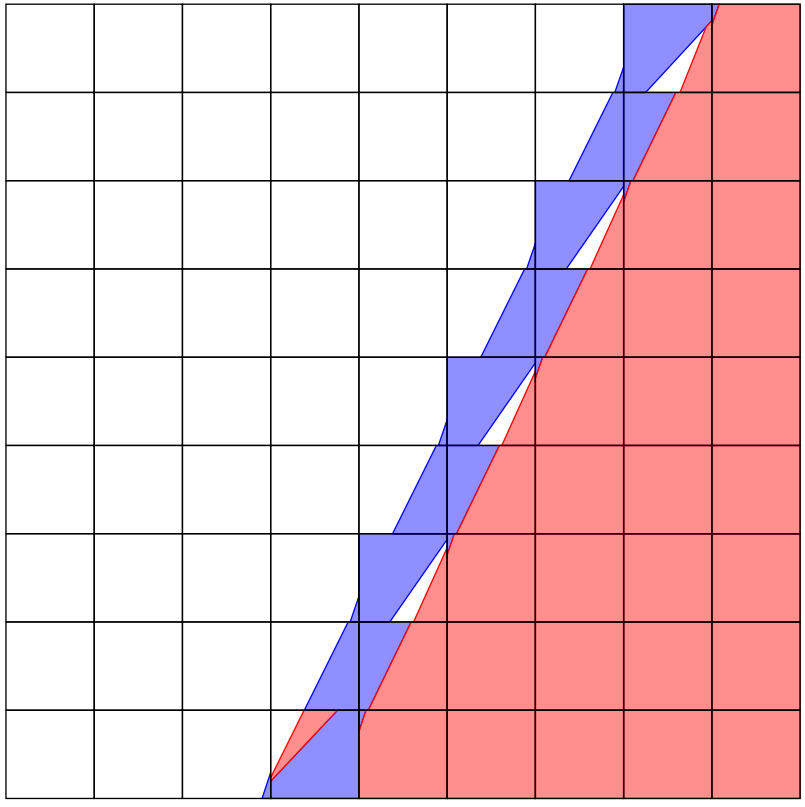
Gradient method
Ordering 2



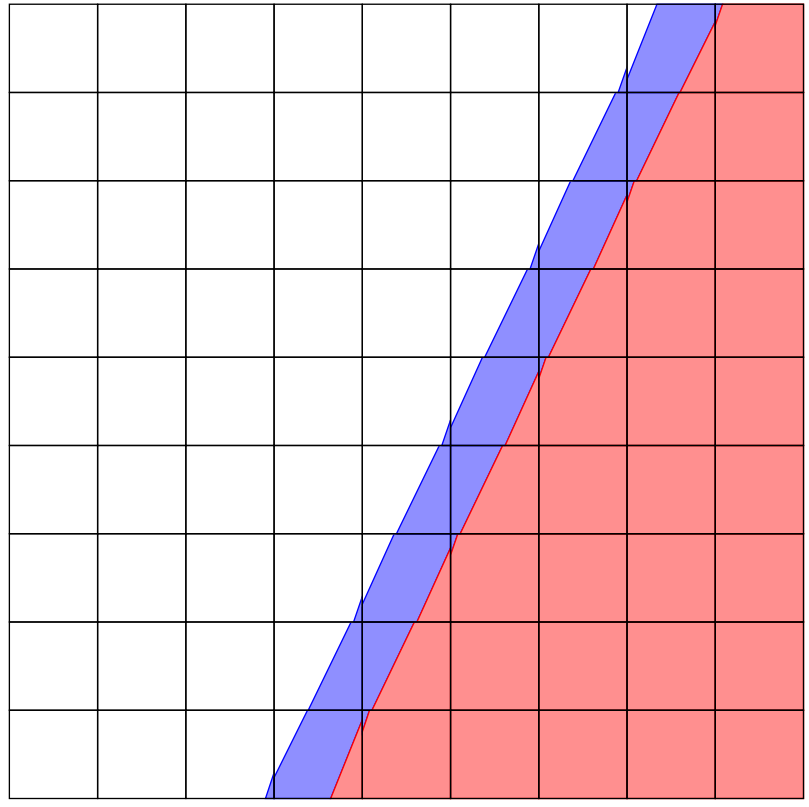
Power Diagram method
Order Independent !



Three-Material Filament

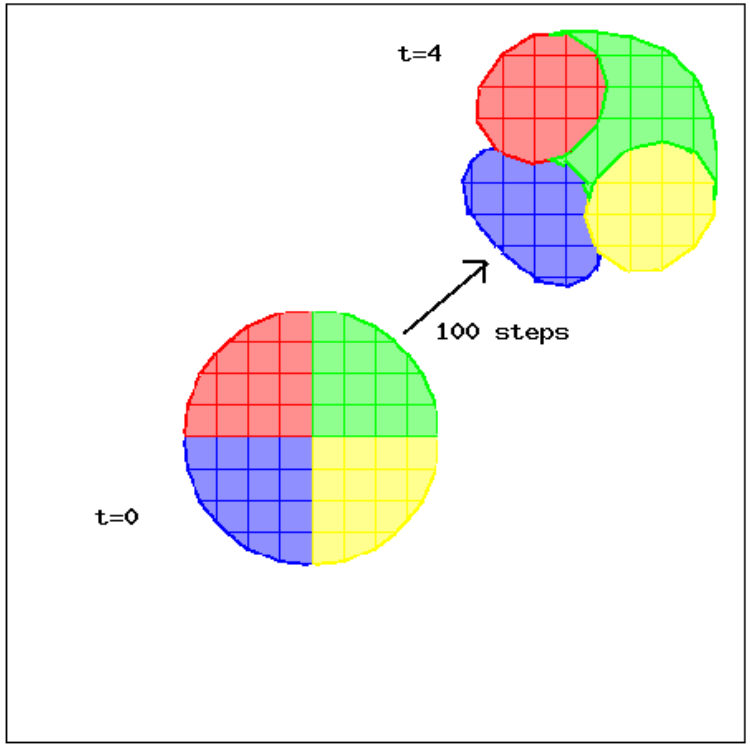


Gradient method
incorrect ordering
(Blue-White-Red)

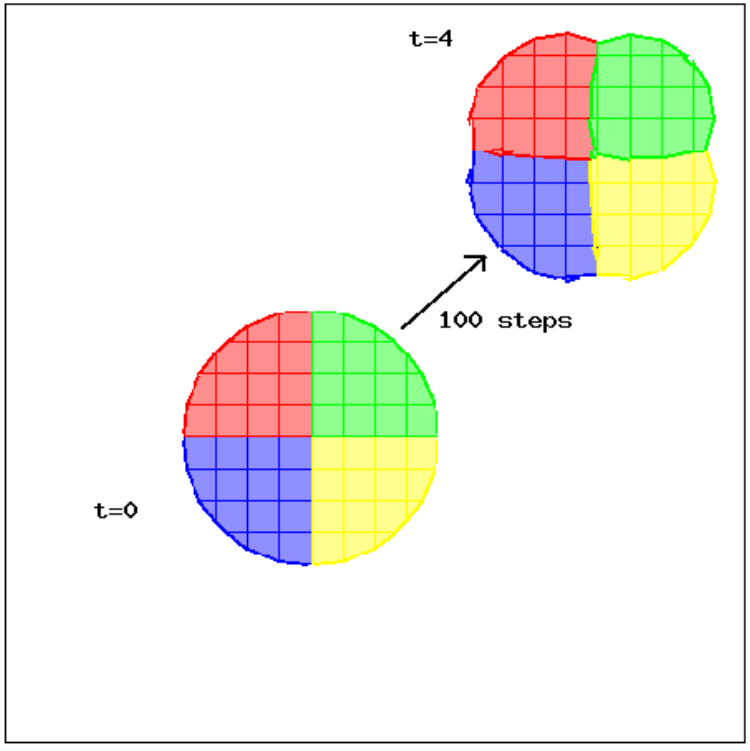


New method
Order-independent

Multi-material Bubble Advection - Comparison of Youngs and VOF-PD



Gradient Method



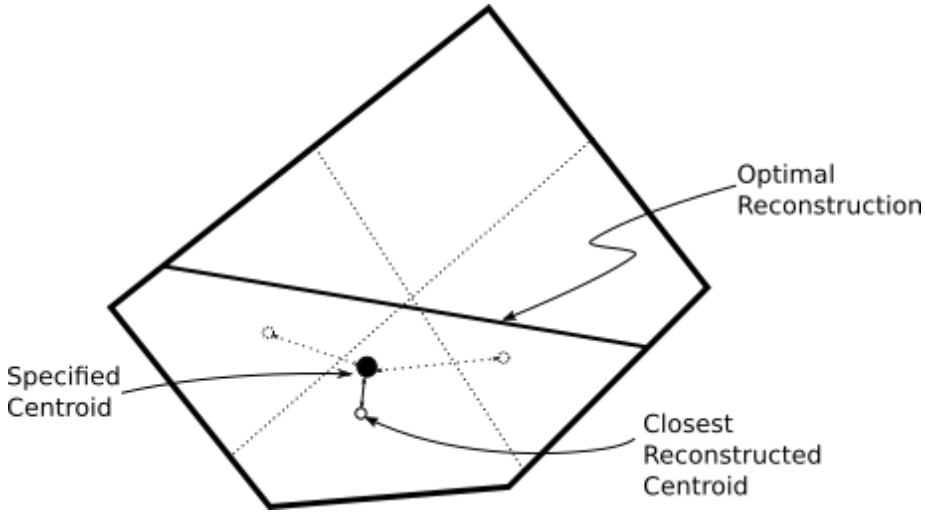
New Method

40x40 grid, Diagonal Movement with velocity of (1.1,1.1)

Moment-of-fluid Method

Moment-of-Fluid Method or MOF

- In addition to tracking volumes, let us track first moment (centroid) of materials in cells (Dyadechko and Shashkov)
- Given the volume fraction and centroid of a material, MOF determines the best line segment that
  - cuts off the exact volume fraction
  - minimizes error between reconstructed and specified material centroids
- The best line segment computed by optimizing with respect to the angle the line segment makes w.r.t the x-axis.

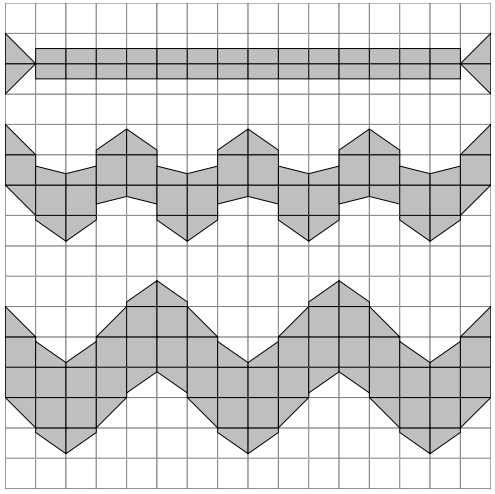


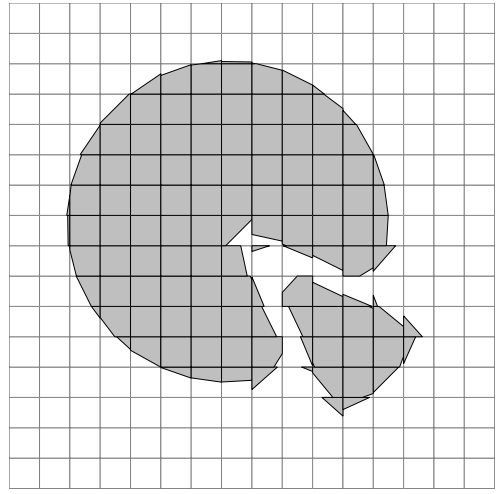
Properties of MOF

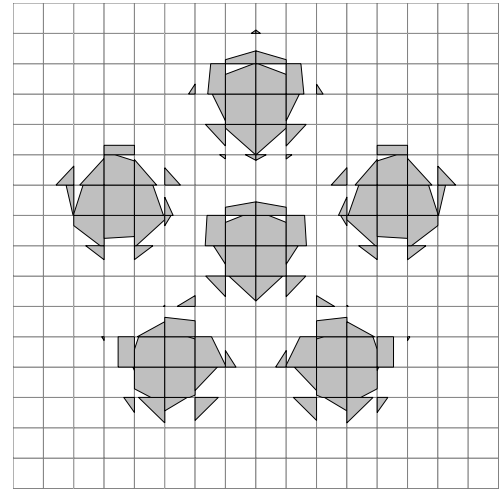
- Second-order accurate
- Local - uses information from only cell under consideration
- Locality is great for parallelization and black-box implementation
- MOF is able to resolve details down to the cell level whereas VOF can only resolve details down to 3-4 local mesh size
- Built-in error estimator - discrepancy between specified and reconstructed centroids
- Error estimate can be used to drive adaptive refinement, automatic material ordering, multi-segmented reconstructions

Static Interface Reconstruction with MOF

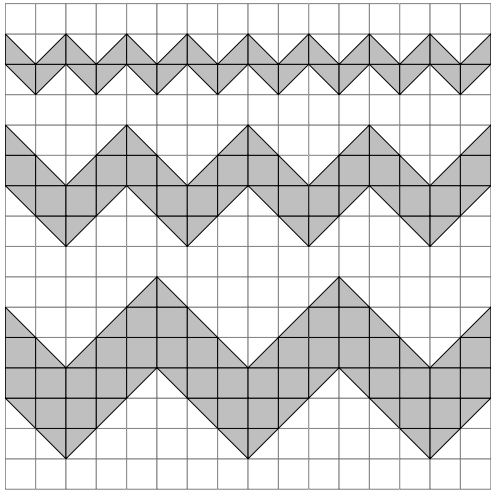
VOF

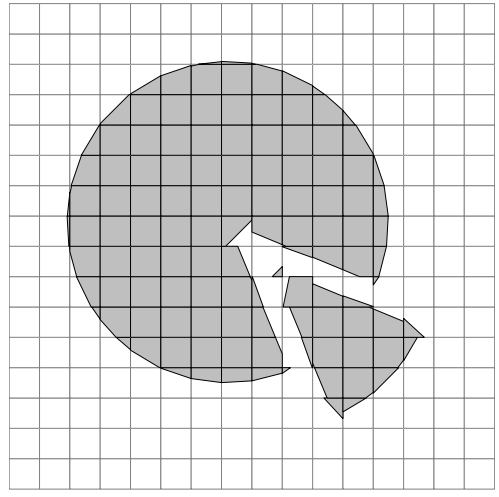


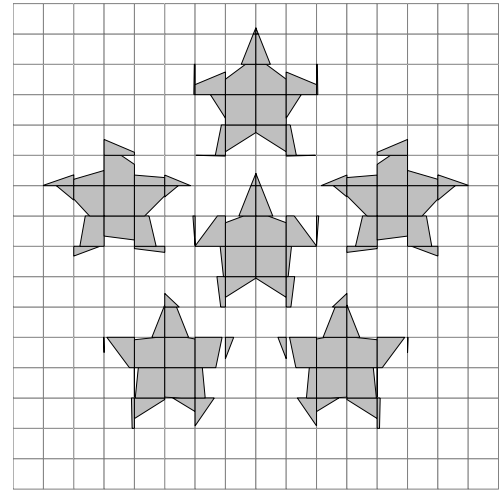




MOF



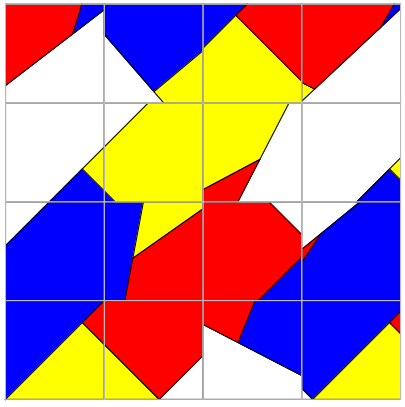


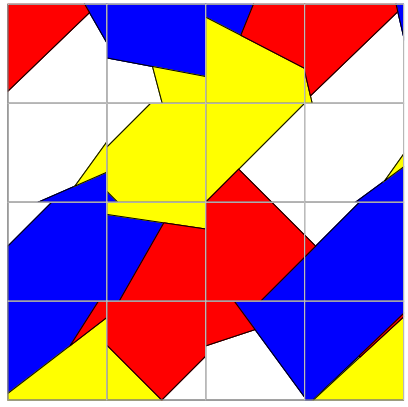


Multi-material Interface Reconstruction

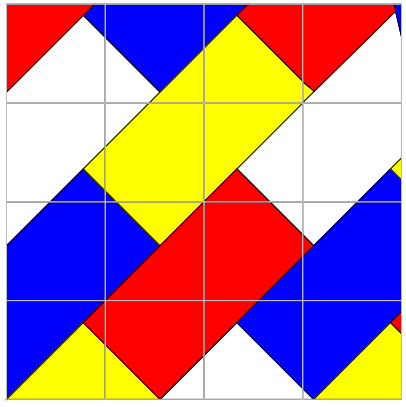
- Compute MOF reconstructions with all possible material orderings ($N!$)
- Choose ordering that minimizes the discrepancy between the reconstructed and specified moments over all materials
- For complex configurations, use a recursive bisection approach
- Choose an arbitrary $n < N$, separate materials $(1, n)$ from $(n+1, N)$, and recursively apply procedure to each subcell containing $2+$ materials
- Procedure effectively generates accurate material order-independent reconstructions

Examples of Multi-material Reconstructions

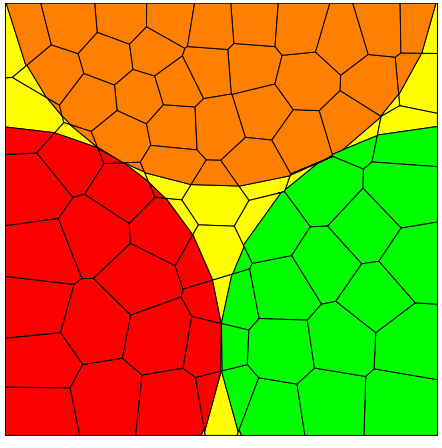


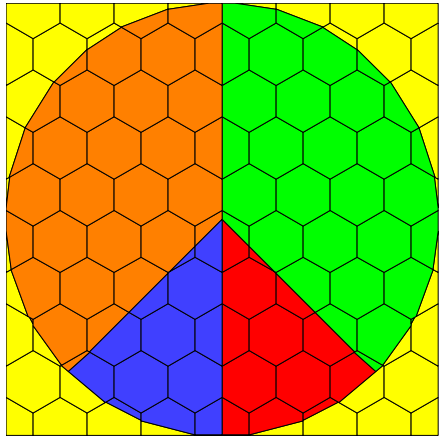


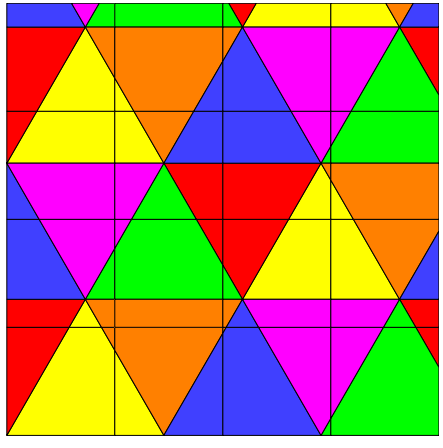
Without automatic material ordering



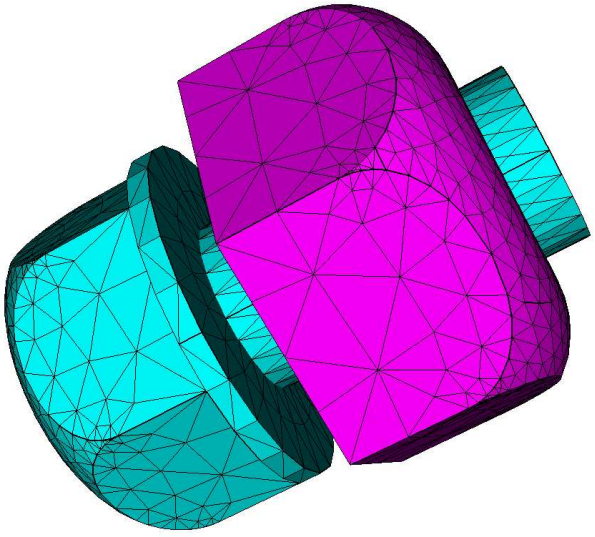
With automatic material ordering

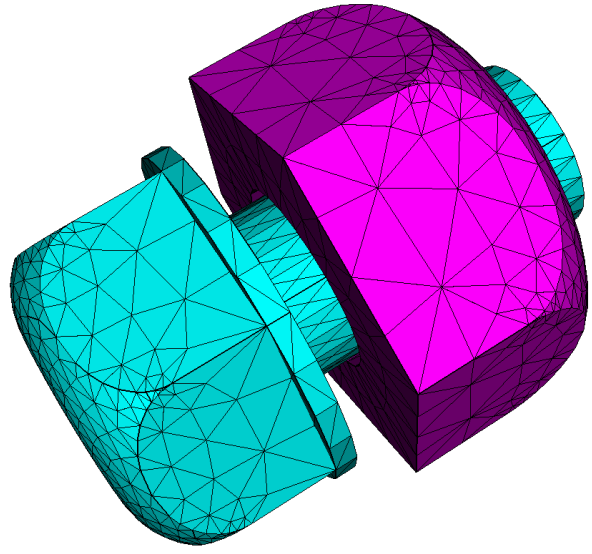


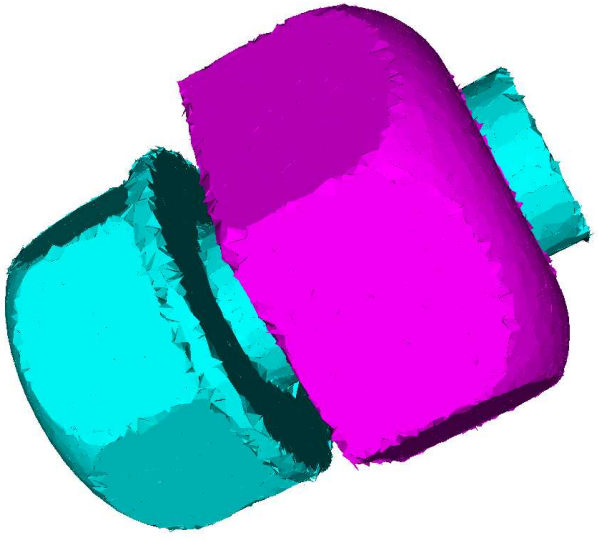


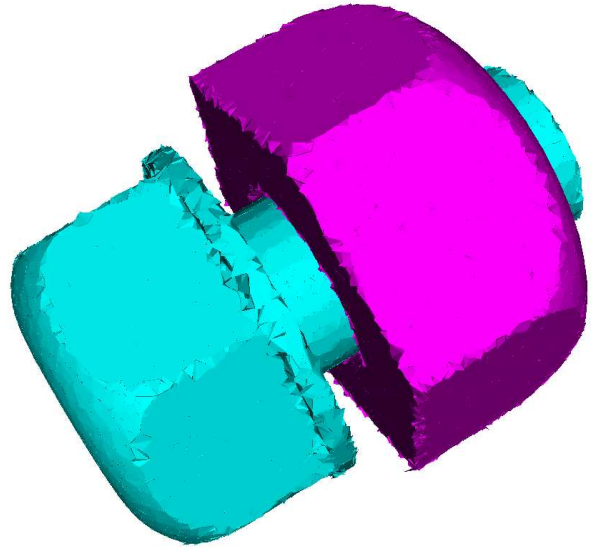


MoF Interface Reconstruction in 3D - Bolt-and-Nut

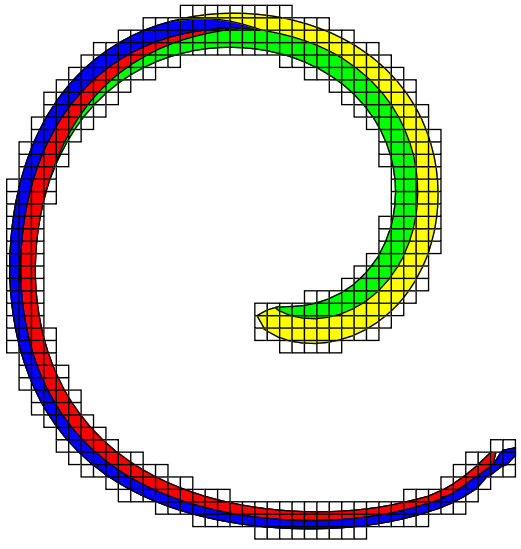




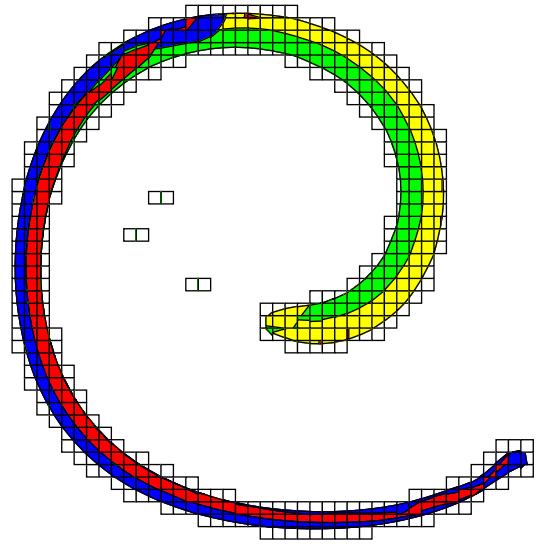




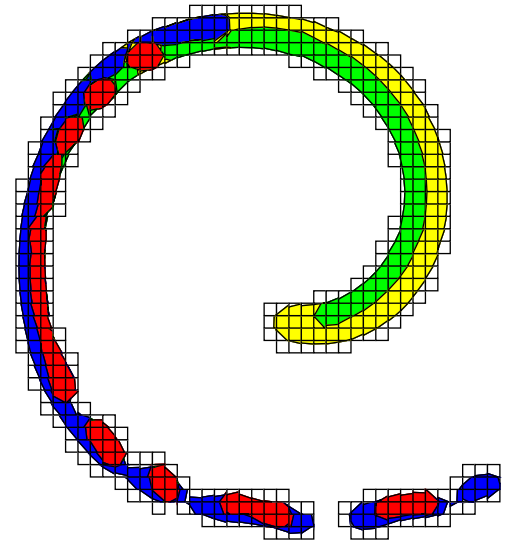
Four Material Vortex-in-a-box Test



MOF



Swartz



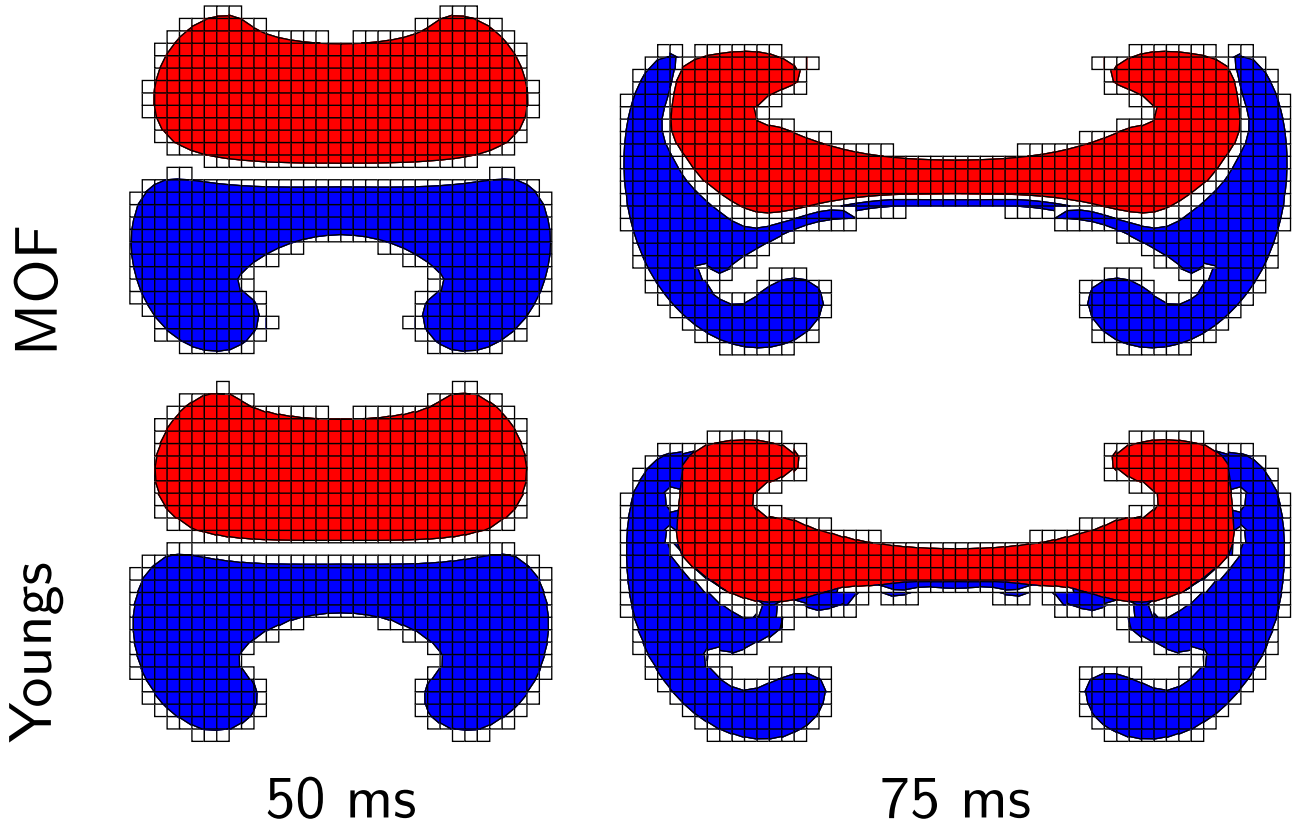
Youngs'

$T = 4$

Colliding bubbles

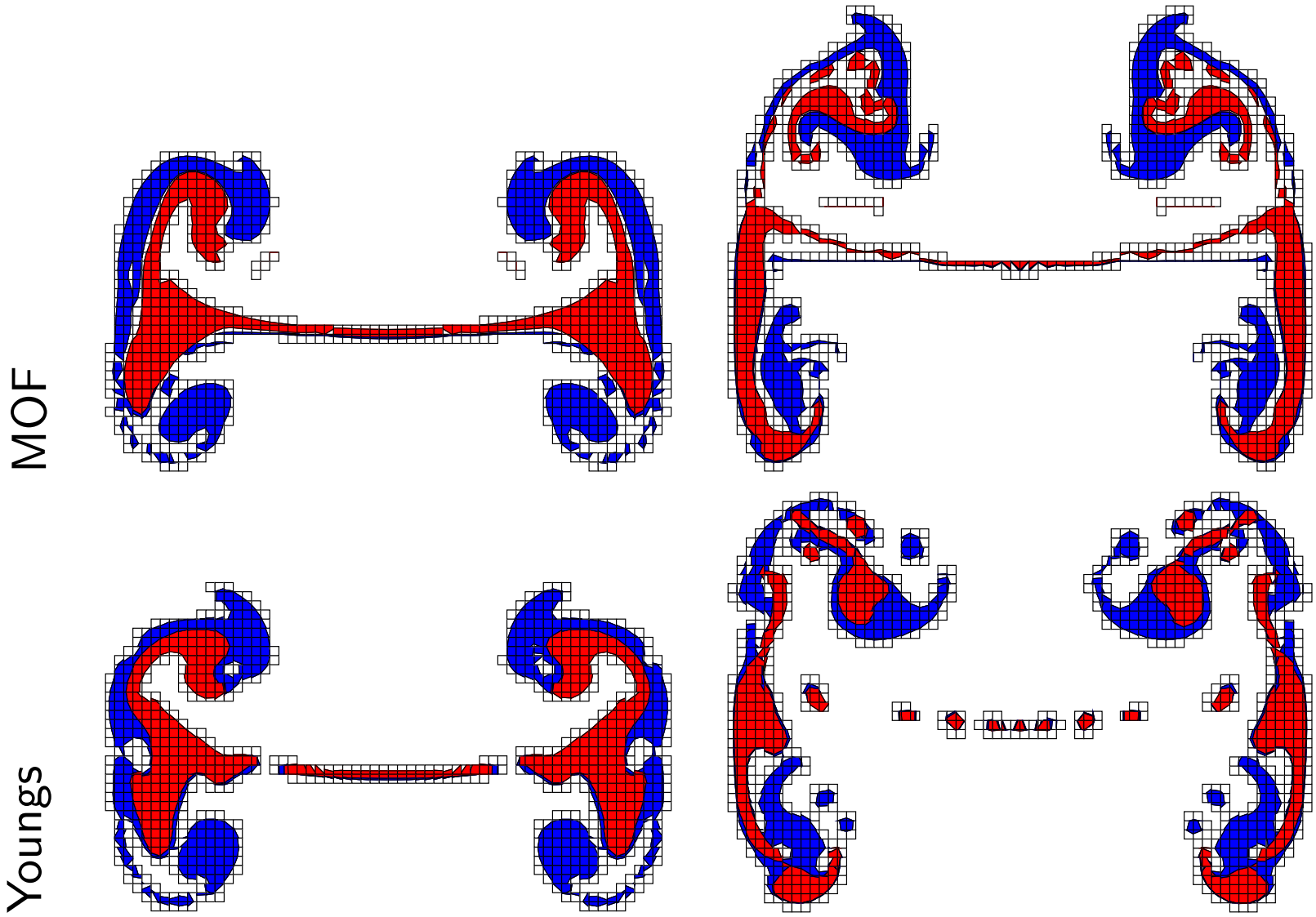
- In this test case, two bubbles of radius 0.15 are in a $[0, 1] \times [0, 2]$ cm tank
- The top bubble has $\rho = 1.5$ g/cm^3
- The bottom bubble has $\rho = 0.5$ g/cm^3 and the ambient fluid has $\rho = 1.0$g/cm^3
- The gravitational force is $g = 981$ cm/s^2 directed along the negative y axis
- Surface tension forces were not present

Colliding bubbles



64×128 grid $\Delta t = 5.0e-4$

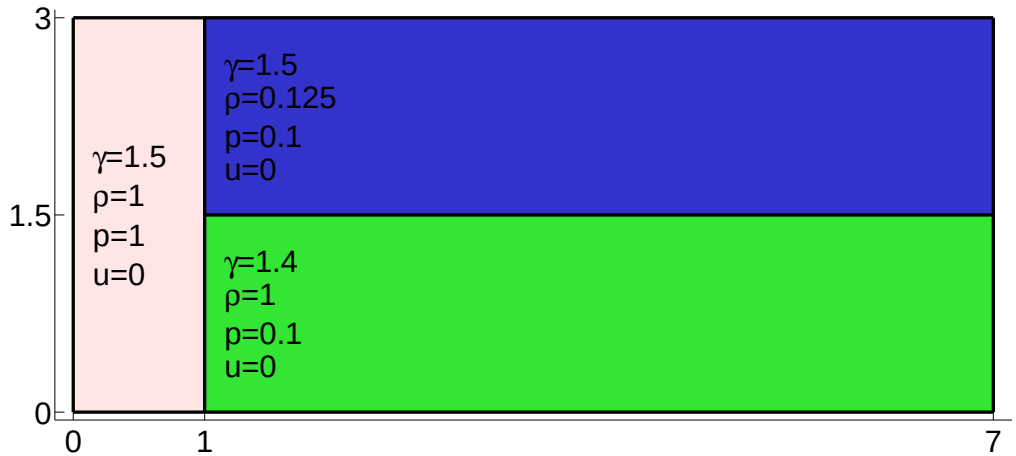
Colliding bubbles - late time

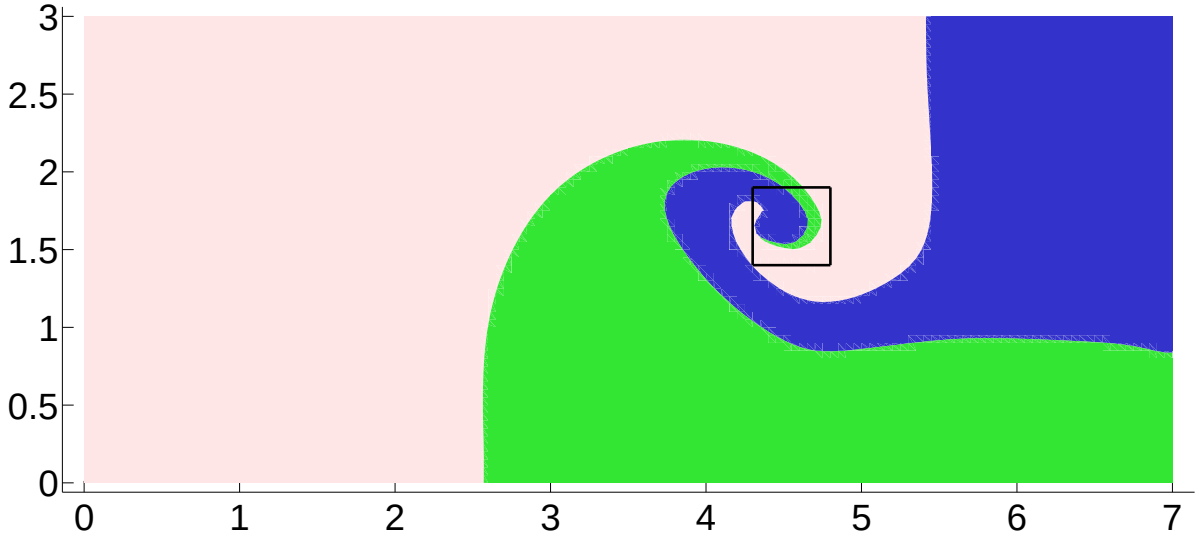


64×128 grid $\Delta t = 5.0e-4$

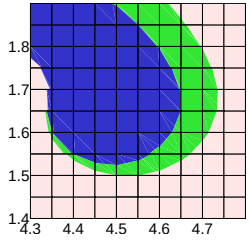
Comparison with ALE Code for Compressible Flows

- Test VOF, VOF-PD and MOF on compressible flow problem
- Rectangular domain of 7x3 units, regular mesh of 140x60
- Three materials at rest, initially forming a T-junction
- The high pressure material (pink) creates a shock wave moving to the right
- Density difference in blue and green materials causes differential shock speed
- Vortex forms around triple point with later stages exhibiting filamentary structures

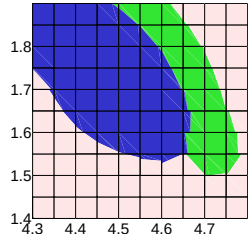




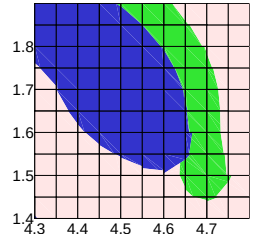
Global view of MOF simulation



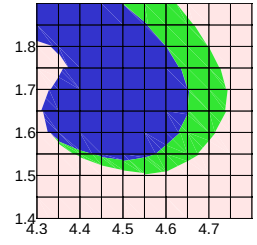
VOF
R first



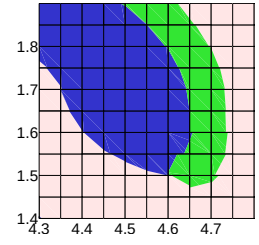
VOF
G first



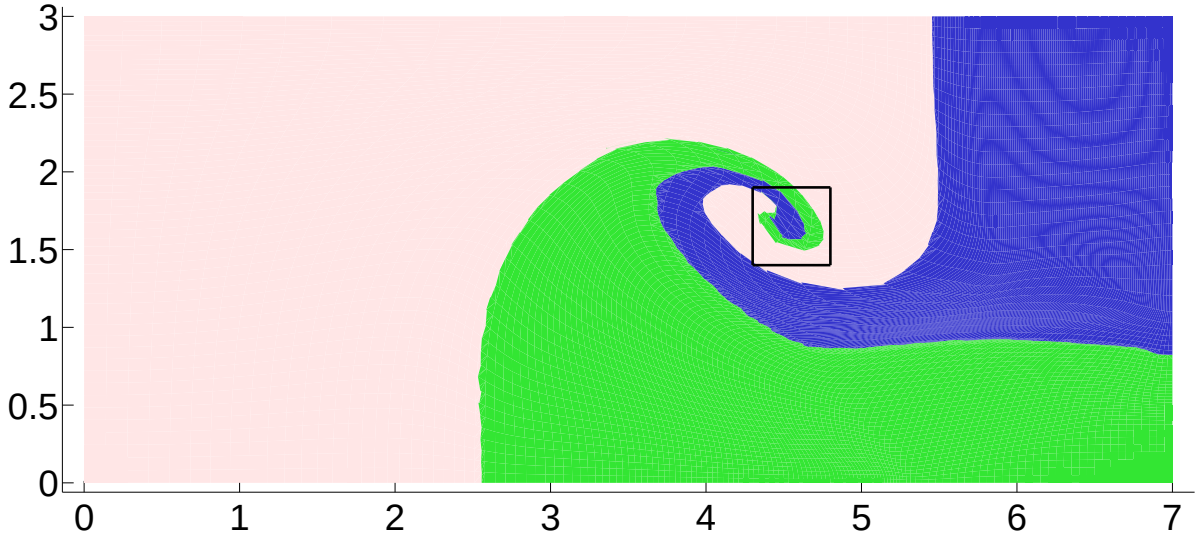
VOF
B first



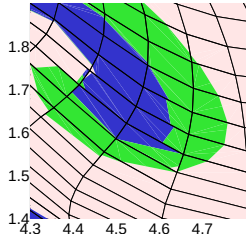
MOF



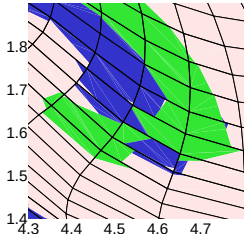
PD



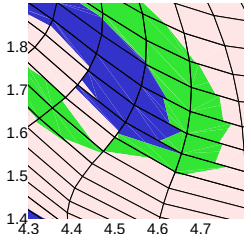
Global view of MOF simulation



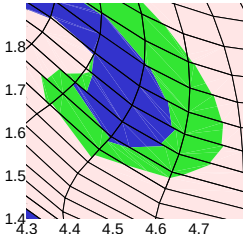
VOF
R first



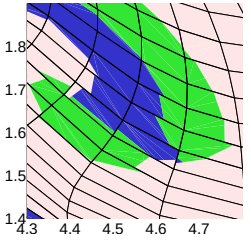
VOF
G first



VOF
B first



MOF



PD

Final Thoughts

- For two material problems, VOF with smoothing is quite good (if there are not many filamentary structures)
- For more than 2 materials, use VOF if the material order is known or trivial to predict
- For complex multi-material problems, use VOF-PD if the advection machinery cannot be revamped
- MOF is the deluxe solution - excellent accuracy, resolution and efficiency, particularly for multi-material problems or problems with thin filaments